Flame Studies of Jet Fuels and Surrogate-Related Neat Components

Chunsheng Ji, Yang Lee Wang, Okjoo Park,
Ning Liu, Ali Moheet, Fokion N. Egolfopoulos

Department of Aerospace and Mechanical Engineering
University of Southern California

MULTI AGENCY COORDINATION COMMITTEE
FOR COMBUSTION RESEARCH (MACCCR)
FUELS RESEARCH REVIEW

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1. **To determine experimentally accurate archival fundamental flame properties (ignition, propagation, extinction) for:**
   - **Selected jet fuels**
   - **Single-component hydrocarbons**
   - **Mixtures of chosen hydrocarbons**

2. **To model experiments using detailed description of chemical kinetics and molecular transport.**

3. **To provide insight into the chemical and physical mechanisms that control the oxidative characteristics of large (liquid) hydrocarbon flames.**

1. **Experimental determination of laminar flame speeds as well as extinction states of atmospheric pressure flames of:**
   - C_5-C_{12} *n*-paraffins (main target: *n*-dodecane)
   - Selected cycloalkanes (main target: *n-butyl*-cyclohexane)
     » Cyclohexane, *methyl*-cyclohexane, *n-butyl*-cyclohexane
   - Selected aromatic compounds (main target: *m*-xylene)
     » Benzene, toluene, *m*-xylene
   - Selected jet fuels (JP-7, JP-8, F-T or S8)

2. **Experimental and numerical capabilities and accuracy were improved notably.**

3. **The accuracy of "standard" measurement techniques was re-evaluated based on evidence produced by experiments, theory, and detailed numerical simulations.**

4. **Insight was gained into the relative importance of the physical and chemical mechanisms that control the flame structure and dynamic behavior.**

1. **Low fuel vapor pressure:**
    - **Fuel heating**
    - **Fuel cracking**
    - **Fuel condensation**
    - **Final mixture composition needs to be tested independent using, e.g., gas chromatography.**
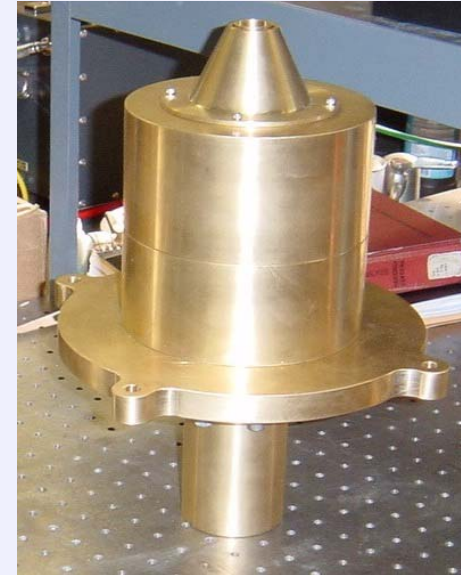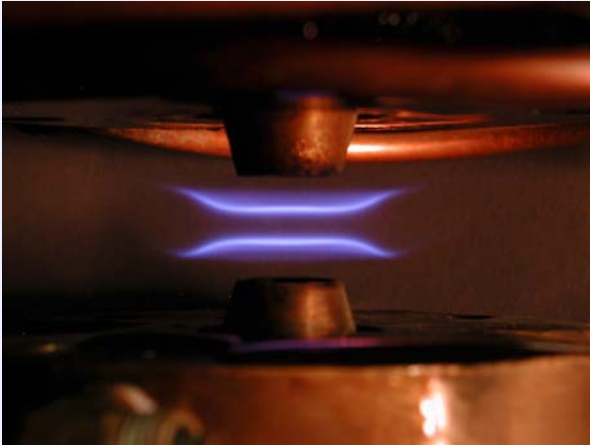
2. **Experiments can be further complicated as pressure increases.**

3. **The large molecular weight discrepancy between fuel and oxidizer can complicate experimental data interpretation.**
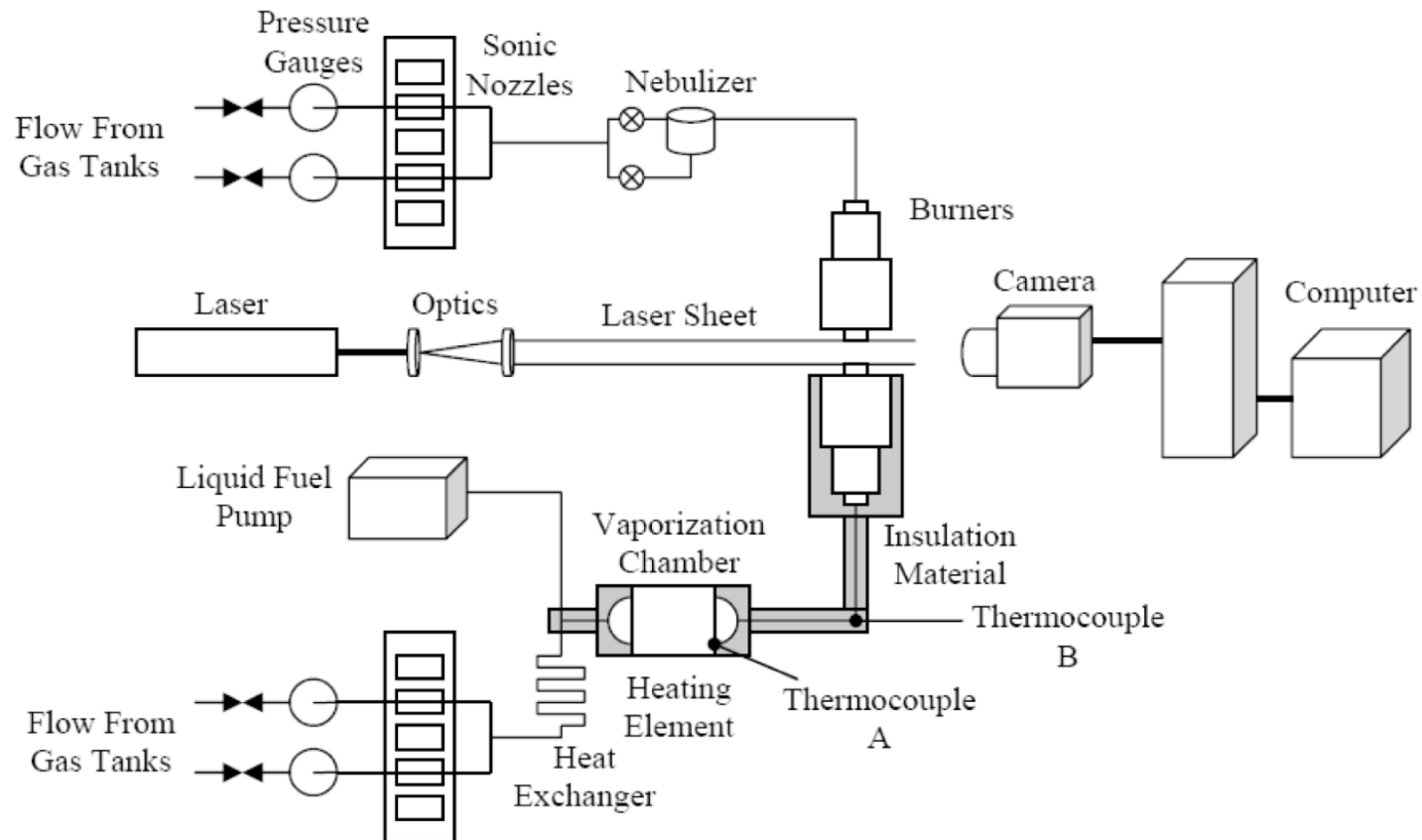
- **Use of counterflow technique (L/D ≤ 1)**

- ○ **Pressure chamber:**
  - **Pressure range 1-10 atm**
- ○ **Diagnostics:**
  - **Laser Doppler Velocimetry (LDV)**
 - **Digital Particle Image Velocimetry (DPIV)**
  - **Thermocouples**

o **Flame stability has improved notably through extensive revisions of:**
  - **Liquid fuel injection**
  - **Silicon oil droplets injection, to perform DPIV measurements**

o **Use of CHEMKIN-based codes**

o **Proper description of "turning-point" behavior**

o **Mathematically rigorous determination of logarithmic sensitivity coefficients: $\partial(\ln Y)/\partial(\ln X)$**

- **Y: laminar flame speed / extinction strain rate / ignition temperature**
- **X: A-factor / D_{i-N2}**

o **Use of JetSurF (http://melchior.usc.edu/JetSurF) kinetic model(s) developed by Wang and coworkers.**

o *All numerical results have been produced by solutions that:*
- *Were properly converged, i.e. in highly resolved grids*
- *Included the effects of thermal radiation and Soret*
- *Included full multi-component transport formulation*
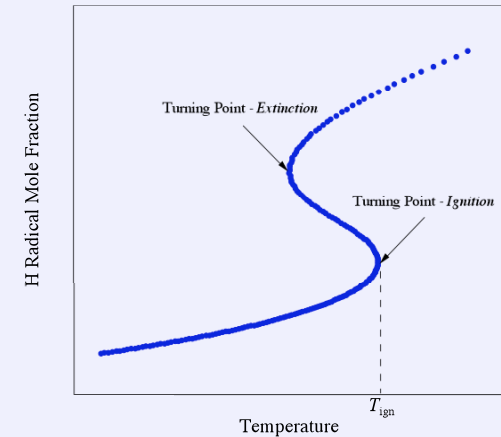
Propagation & Extinction
Holley et al. 32nd Symposium
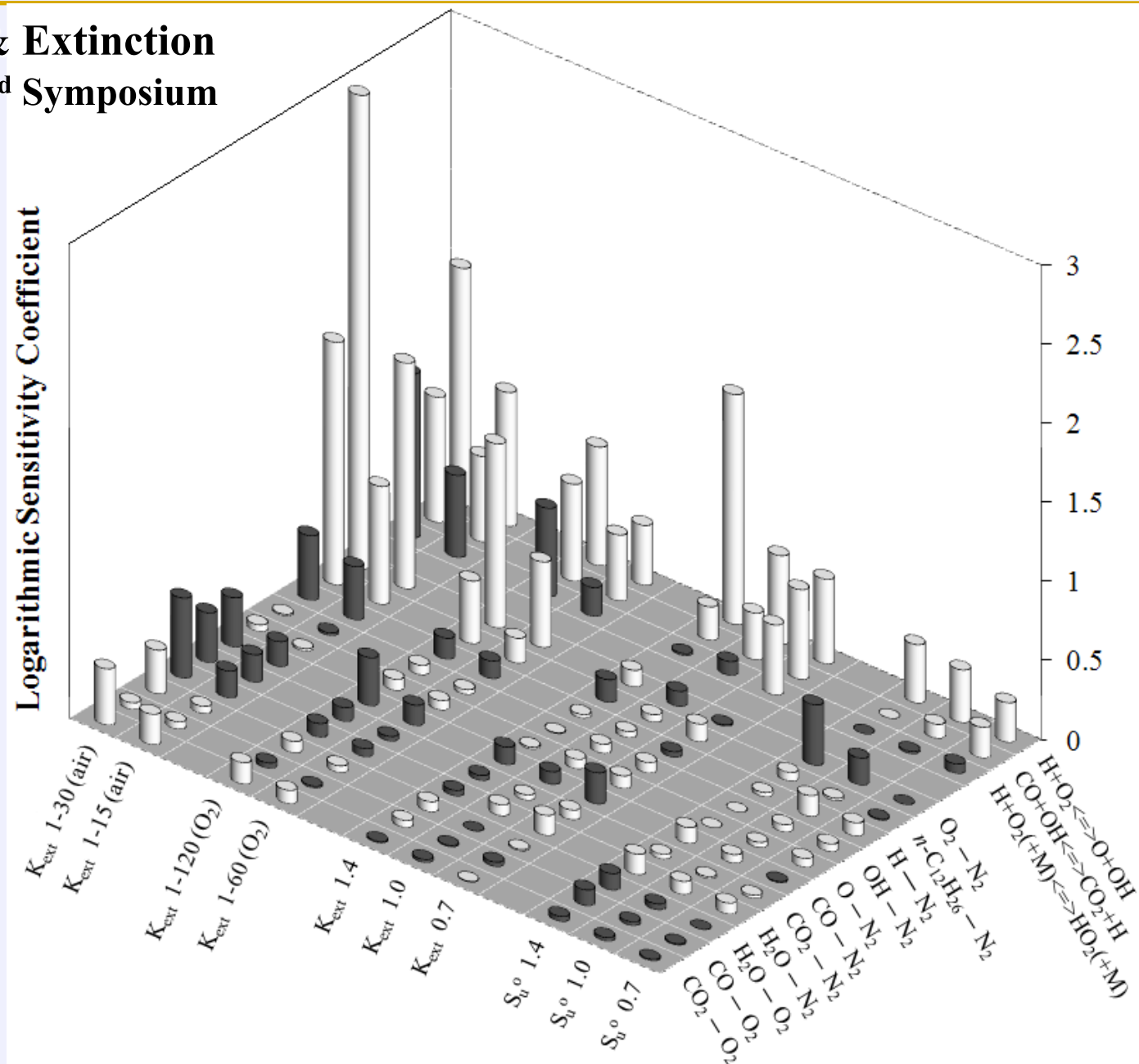
Ignition of premixed flames:
$C_{12}H_{26}$/air (ϕ=0.7) against hot N_2
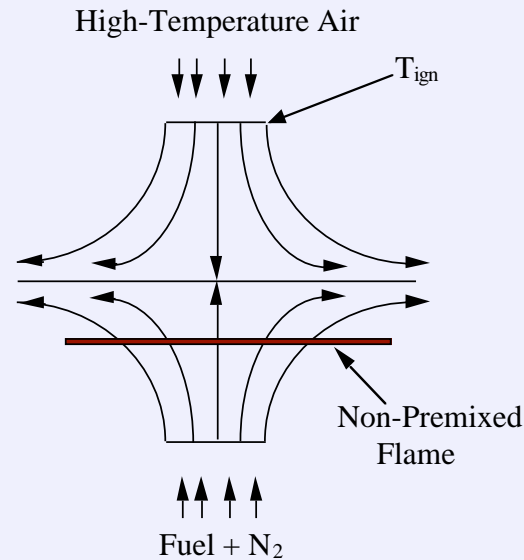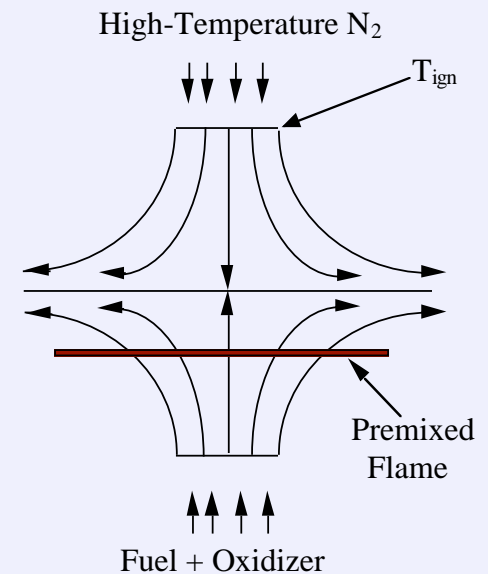
(Unpublished work)

Premixed Flame Ignition
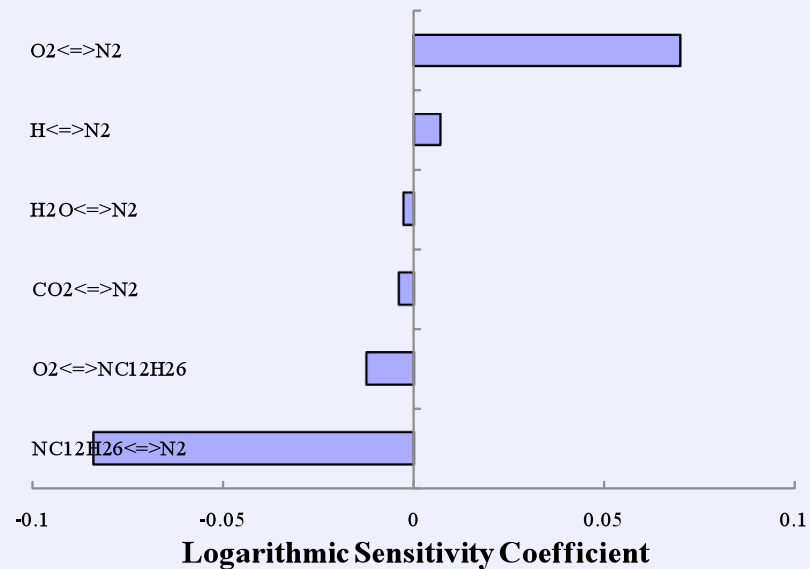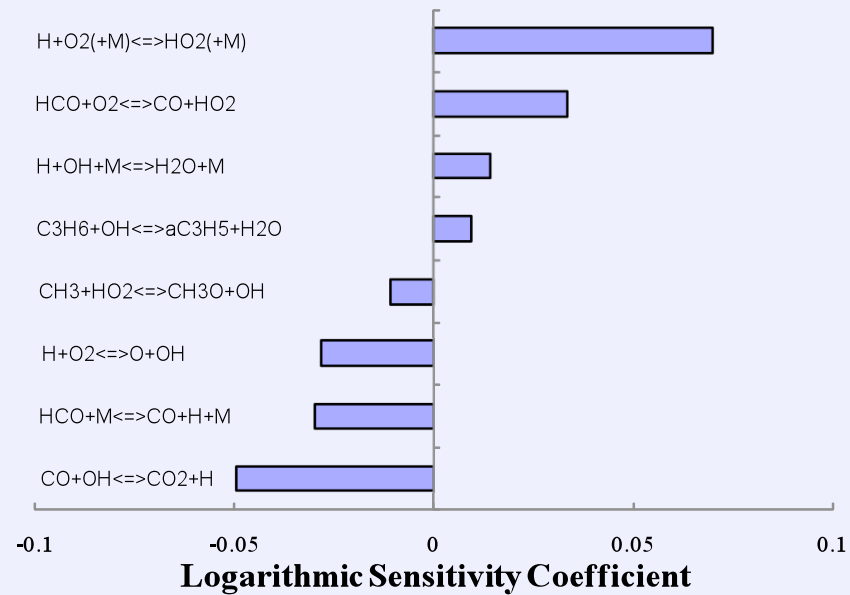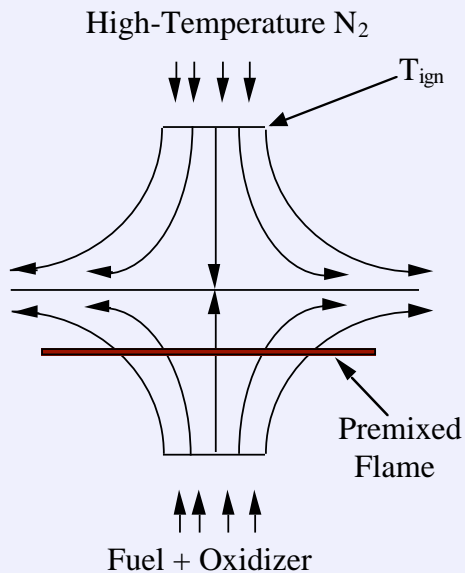
High-Temperature N_2

T_{ign}

Premixed
Flame

Fuel + Oxidizer

Logarithmic Sensitivity Coefficient

H+O2(+M)<=>HO2(+M)
HCO+O2<=>CO+HO2
H+OH+M<=>H2O+M
C3H6+OH<=>aC3H5+H2O
CH3+HO2<=>CH3O+OH
H+O2<=>O+OH
HCO+M<=>CO+H+M
CO+OH<=>CO2+H

-0.1   -0.05   0   0.05   0.1

Logarithmic Sensitivity Coefficient

O2<=>N2
H<=>N2
H2O<=>N2
CO2<=>N2
O2<=>NC12H26
NC12H26<=>N2

-0.1   -0.05   0   0.05   0.1

Non-Premixed Flame Ignition

High-Temperature Air

T_{ign}

Non-Premixed Flame

Fuel + N_2

Premixed Flame Ignition

High-Temperature N_2

T_{ign}

Premixed Flame

Fuel + Oxidizer

o **Special care to establish:**

- **As uniform as possible exit temperature profile**

- **As uniform as possible exit velocity profiles**

- **As stable as possible flow-field**

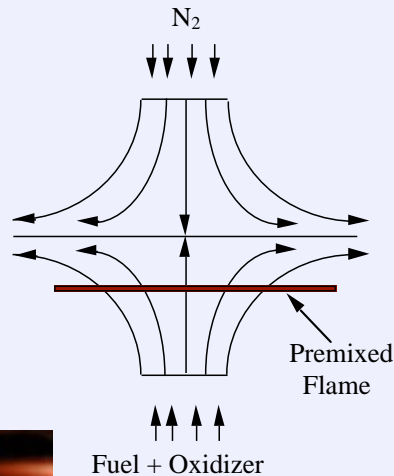o **Non-premixed vs. premixed flame ignition: Why?**
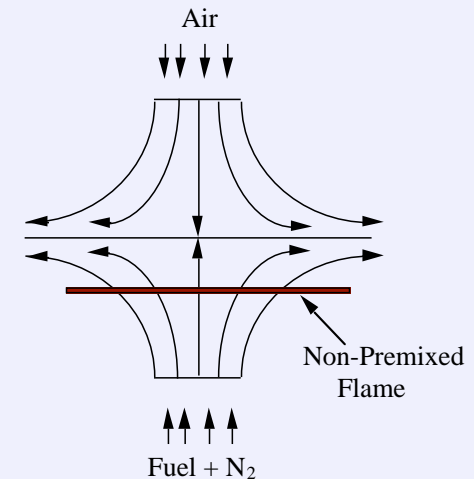
Premixed Twin Flame Extinction
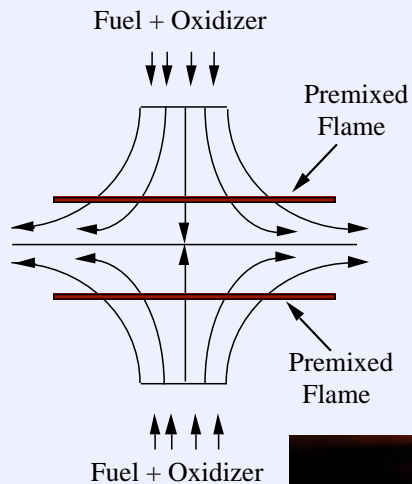
Premixed Single Flame Extinction

Non-Premixed Flame Extinction

Fuel + Oxidizer

Premixed Flame

Premixed Flame

Fuel + Oxidizer

N_2

Premixed Flame

Fuel + Oxidizer

Air

Non-Premixed Flame

Fuel + N_2

o **The (extinction) strain rate is determined as the maximum axial velocity gradient upstream of the flame**

o **No extrapolations are performed**

o **The injection velocity gradient is recorded also, as it is an essential input into the simulations**
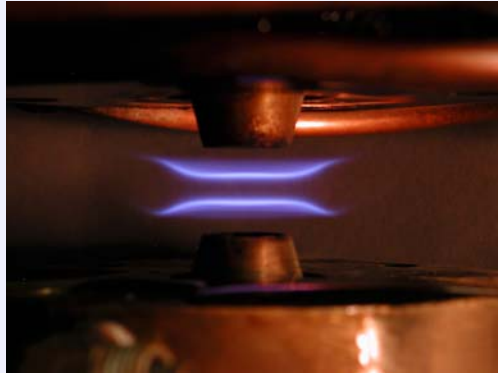
Premixed Twin Flame Extinction

Fuel + Oxidizer

Premixed Flame

Premixed Flame

Fuel + Oxidizer
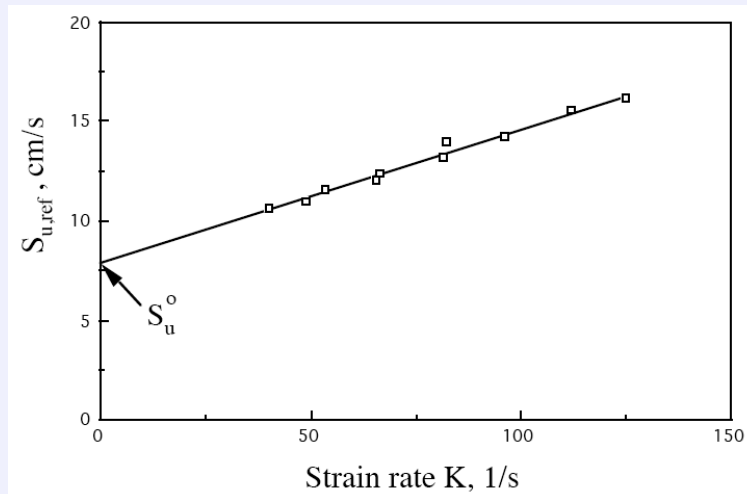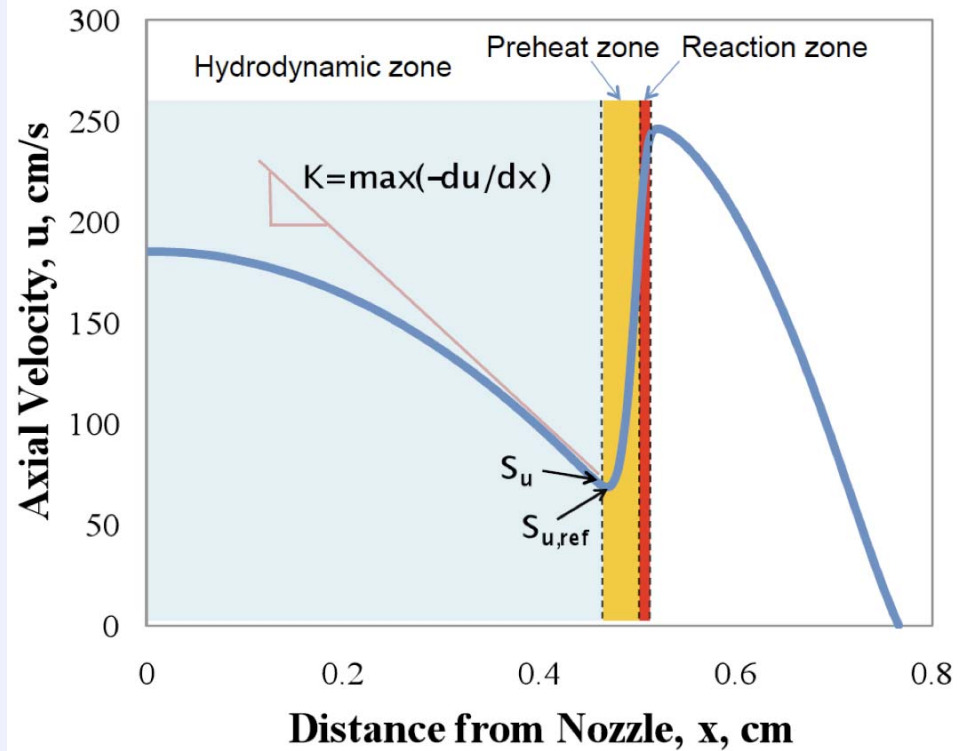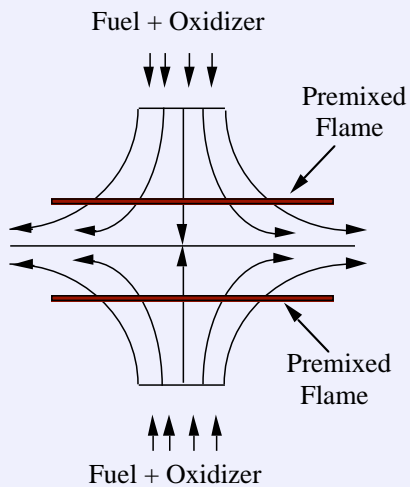
o **Current approaches:**
  - **Spherically expanding flames (SFEs) in constant P or V chambers.**
  - **Stagnation flames (SFs)**
  - **Bunsen flames**

o **Key advantages:**
  - **Spherically expanding flames:**
    - ➤ **Well defined stretch**
    - ➤ **Fast experiment, small fuel quantities needed**
    - ➤ **Easily implemented in high pressures**
  - **Stagnation flames:**
    - ➤ **Well defined stretch**
    - ➤ **Easily probed with laser diagnostics, direct measurements can be made**

o **Key disadvantage for both SFs and SFEs:**
  - **The zero stretch state cannot be reached experimentally so that extrapolations are needed.**

- **Traditionally:**

  ➤ **Linear extrapolation:** $S_u = S_u^o + \mu k$
  Overpredicts the laminar flame speed

  ➤ **Non-linear extrapolation (based on asymptotic analysis)[1]**
  $$S_{u,ref} = S_u^o\{1-(\mu-1)Ka+Ka\ln[(\sigma-1)Ka]\}$$

  - One-step, one-reactant chemistry
  Assumptions: - Constant μ, λ, c_p, D
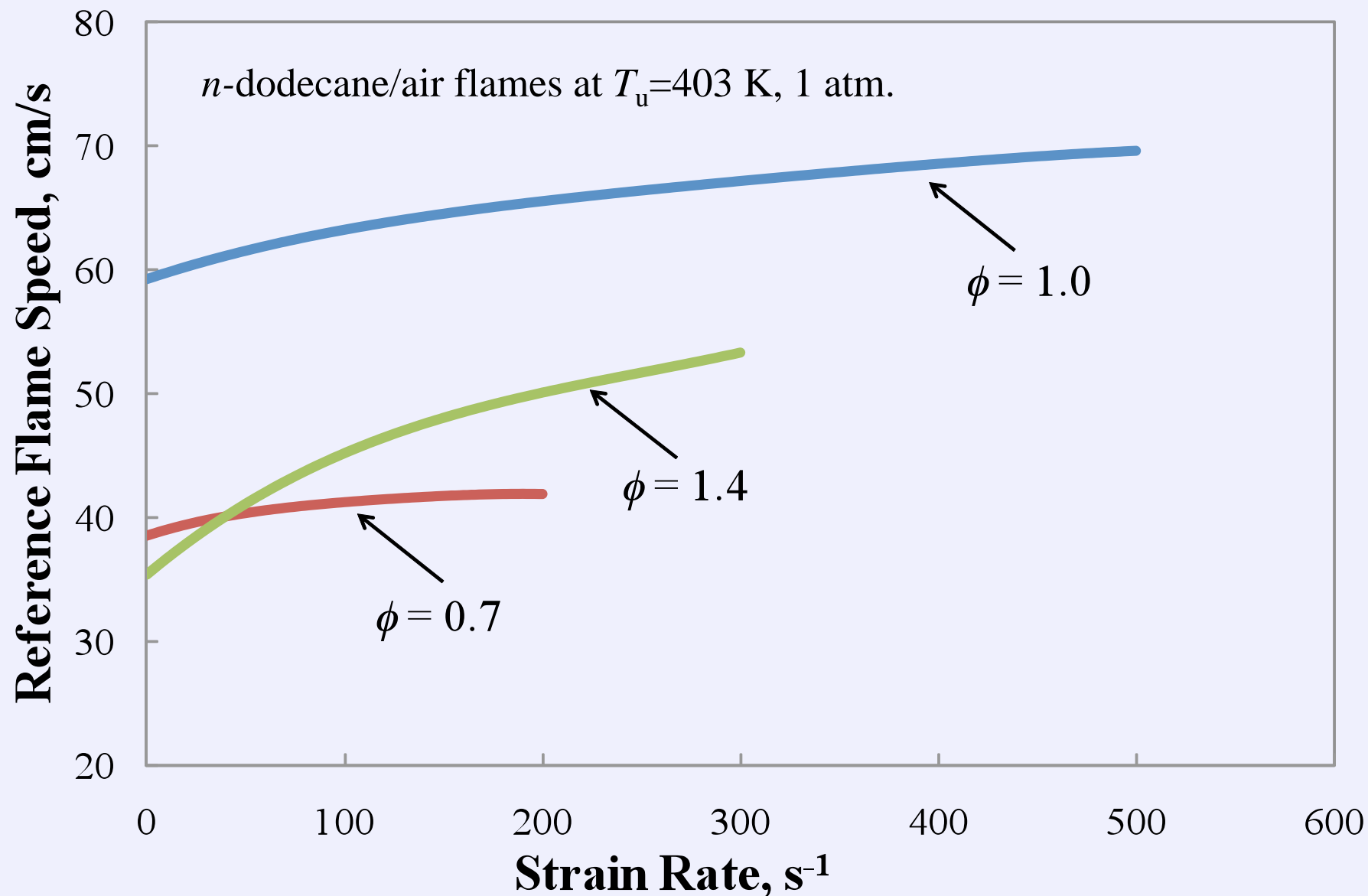 - Infinite domain

- **New computationally-assisted extrapolation approach[2]**
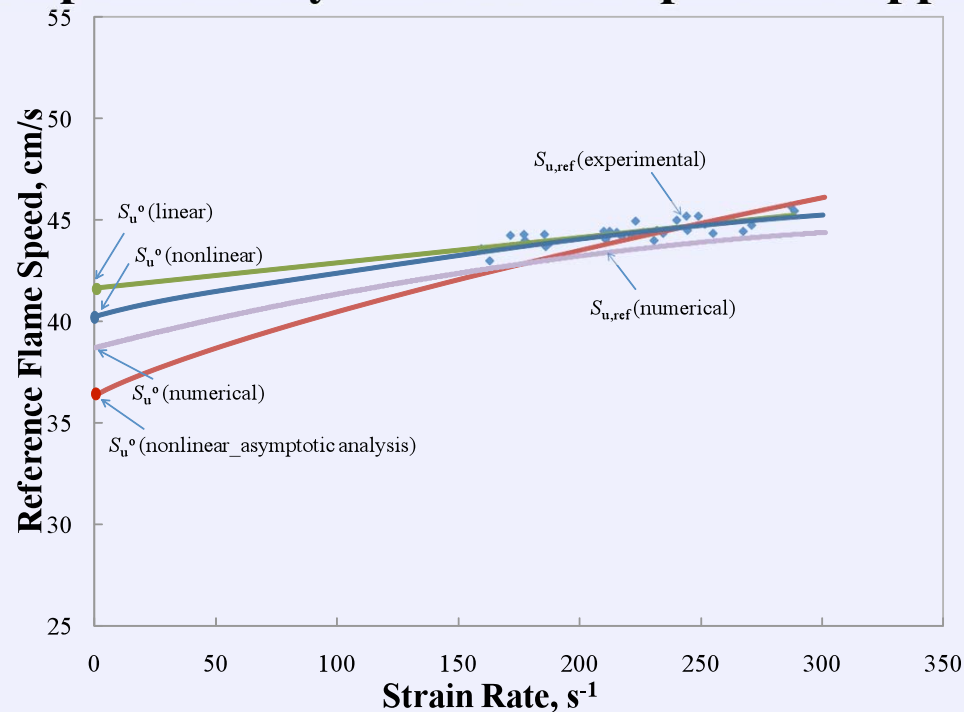
[1] J. H. Tien, M. Matalon, Combust. Flame 84(3-4) (1991) 238-248
[2] Y. L. Wang, A. T. Holley, C. Ji, F. N. Egolfopoulos, T. T. Tsotsis, H. J. Curran, Proc. Combust. Inst. 32 (2009) 1035-1042

n-dodecane/air flames at T_u=403 K, 1 atm.

$\phi = 1.0$

$\phi = 1.4$

$\phi = 0.7$

Reference Flame Speed, cm/s

Strain Rate, s^{-1}

Average difference between linear and nonlinear extrapolation methodology for C_5-C_{12} n-alkane/air flames.
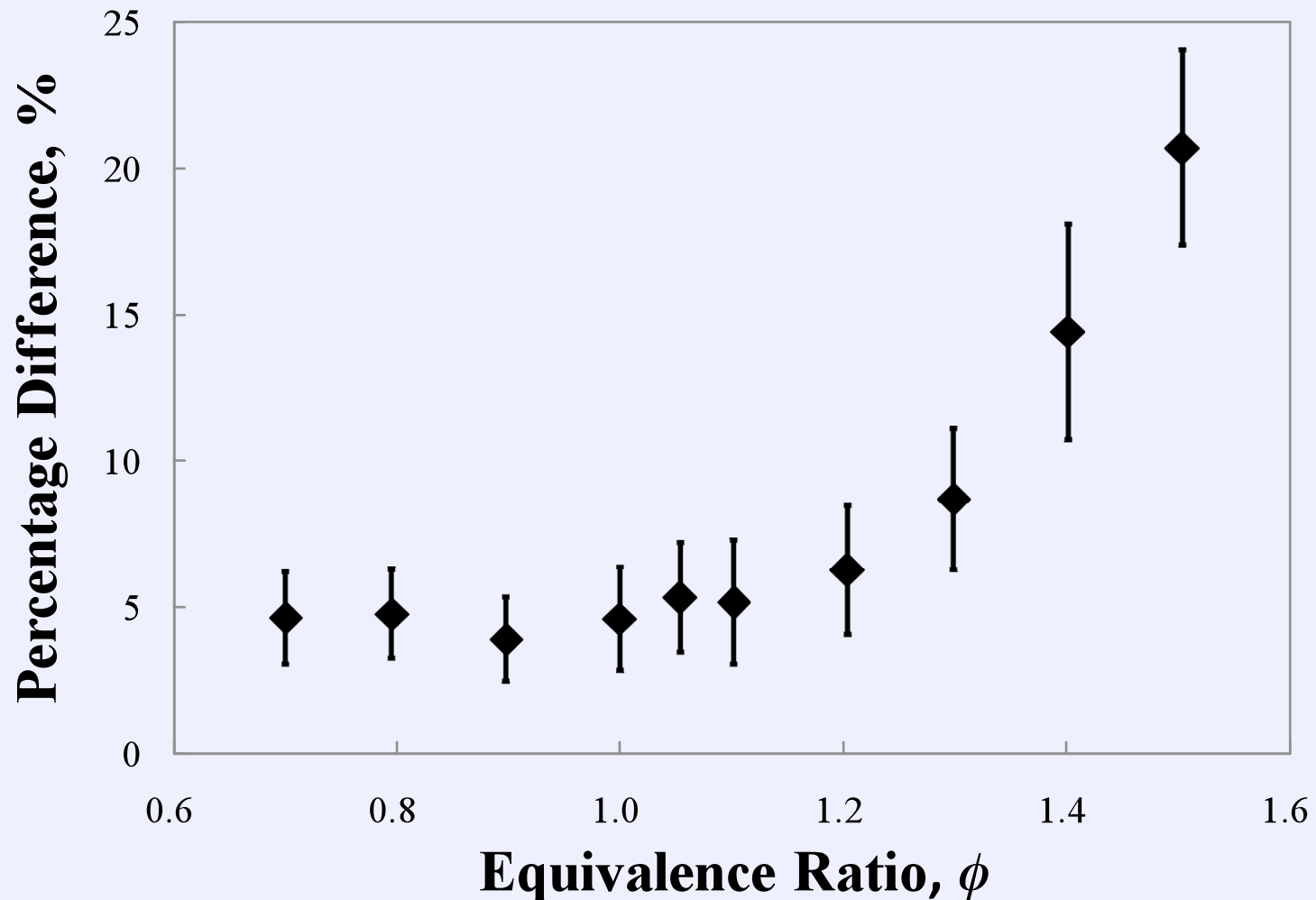
o The shape of the computationally-assisted non-linear extrapolation $S_{u,ref}$ vs. K curve was found to be insensitive (to the first order) to:
   - Small by finite uncertainties in kinetics.
   - Small by finite uncertainties in transport coefficients.
   - Notable imbalance of the momenta of the two impinging jets.
   - Notable changes of the velocity gradient at the nozzle exit.
   - Gross modifications of the combustion chemistry, which however result in the same laminar flame speed.

o WHY?

o For flames established in a finite domain opposed-jet flow-field, their response (including $S_{u,ref}$) to the imposed strain rate K is controlled by the:
   - Size of the finite domain, i.e. the nozzle separation distance L – affects the strain rate distribution inside the transport and reaction zones
   - The flame thickness – affects the magnitude of Karlovitz number
   - The flame temperature – affects kinetics

Notable imbalance of the momenta of the two impinging jets

Notable changes of the velocity gradient at the nozzle exit

Gross modifications of the combustion chemistry, which however results in the same laminar flame speed

n-dodecane/air flame ($\phi = 1.0$) at T_u=403 K, 1 atm

(Chart axes: Reference Flame Speed, cm/s vs Strain Rate, s^{-1})

Curve labels: $(k_{R1}*2, k_{R2})$, (k_{R1}, k_{R2}), $(k_{R1}*2, k_{R2}/3.2)$

$$H + O_2 = OH + O \qquad (R1)$$

$$CO + OH = CO_2 + H \qquad (R2)$$

Gross modifications of the combustion chemistry, which however results in the same laminar flame speed

n-dodecane/air flame ($\phi = 1.0$) at T_u=403 K, 1 atm

H + O$_2$ = OH + O   (R1)

CO + OH = CO$_2$ +H   (R2)
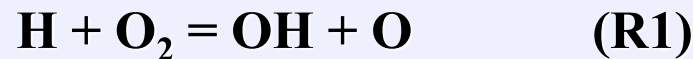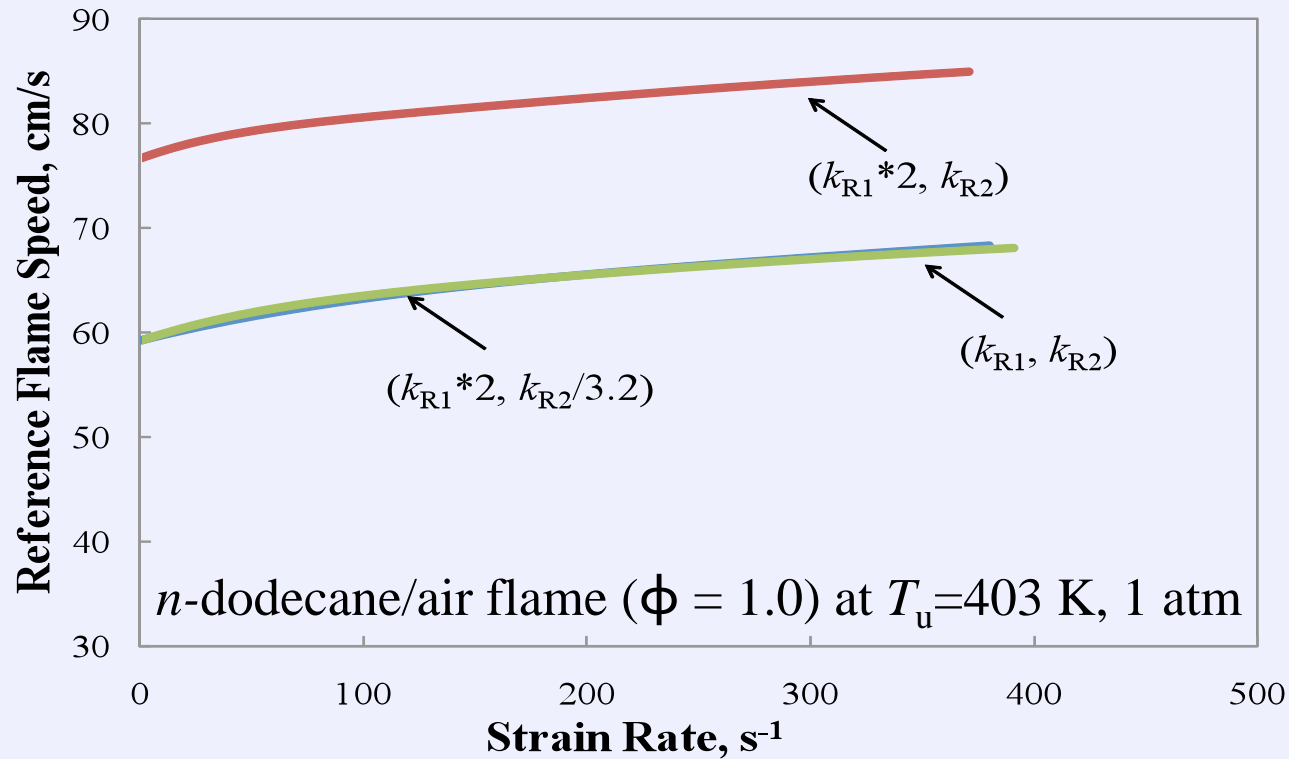
o **Can kinetic models be validated against the raw experimental $S_{u,ref}$ vs. K data obtained in the opposed jet configuration?**

- **YES, if the quasi-1-D code (e.g. OPPDIF) is a reliable representation of the experimental data.**

o **Can a quasi 1-D or full axisymmetric 2-D simulation capture exactly ALL details of the actual experiment?**

- **NO, due to unquantified subtleties of the boundary conditions that cannot be defined with the greatest accuracy so that certain discrepancies can be realized, especially in the flame location.**

o **Can a quasi 1-D or a fully axisymmetric 2-D simulation capture closely the response of the flame to K as observed in experiments? Are 1-D and 2-D simulations consistent in that respect?**

- **YES, based on experimental evidence.**
- **Direct 2-D numerical simulations are currently under way (Pitsch).**

o **Experimental evidence**
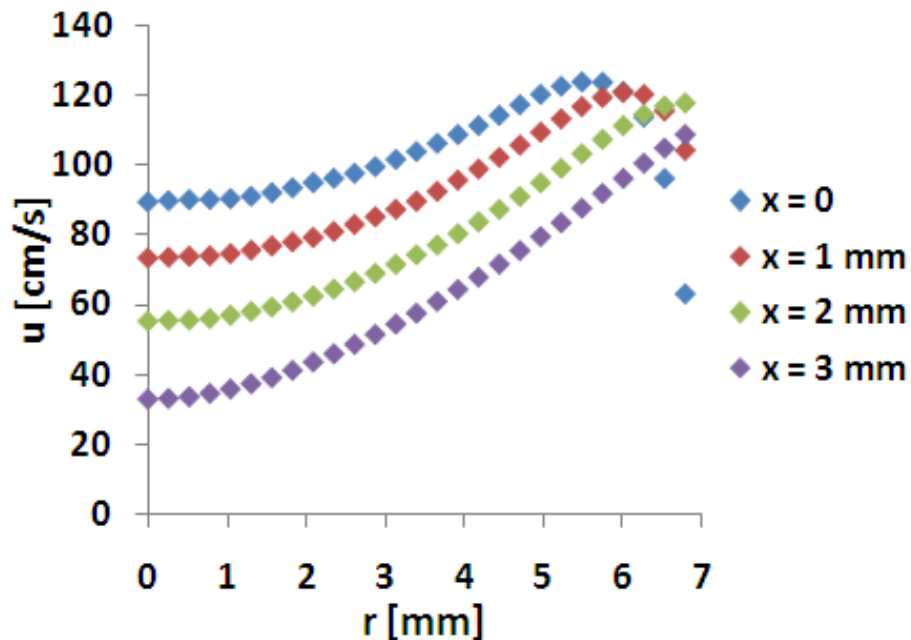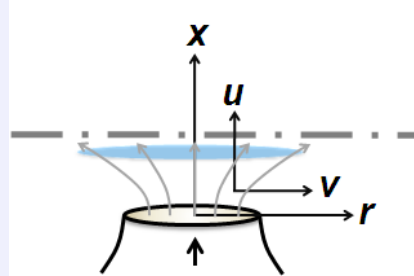
Plug flow assumption valid in core around centerline
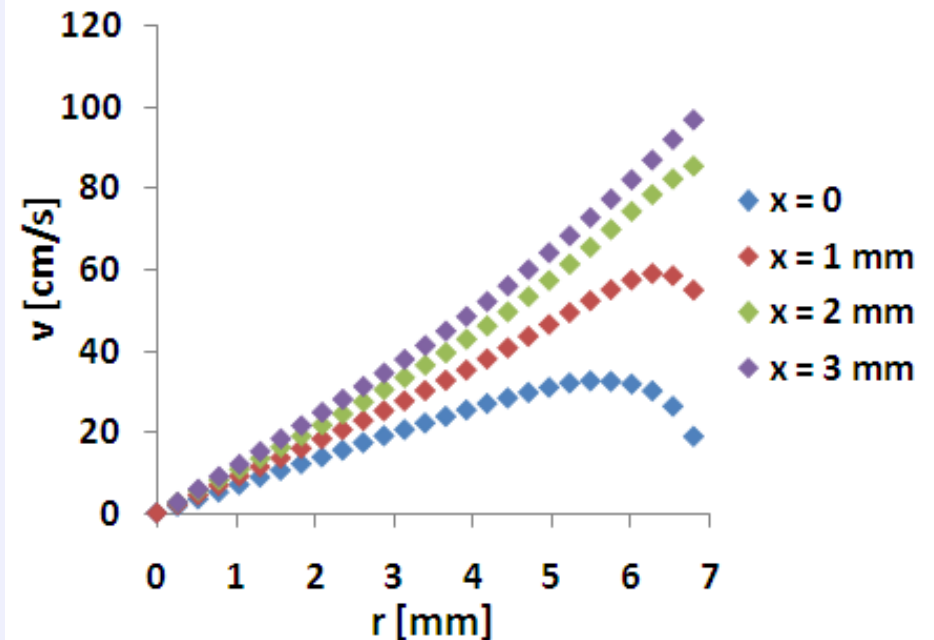
Radial velocity increases linearly with radius

o **Experimental evidence**
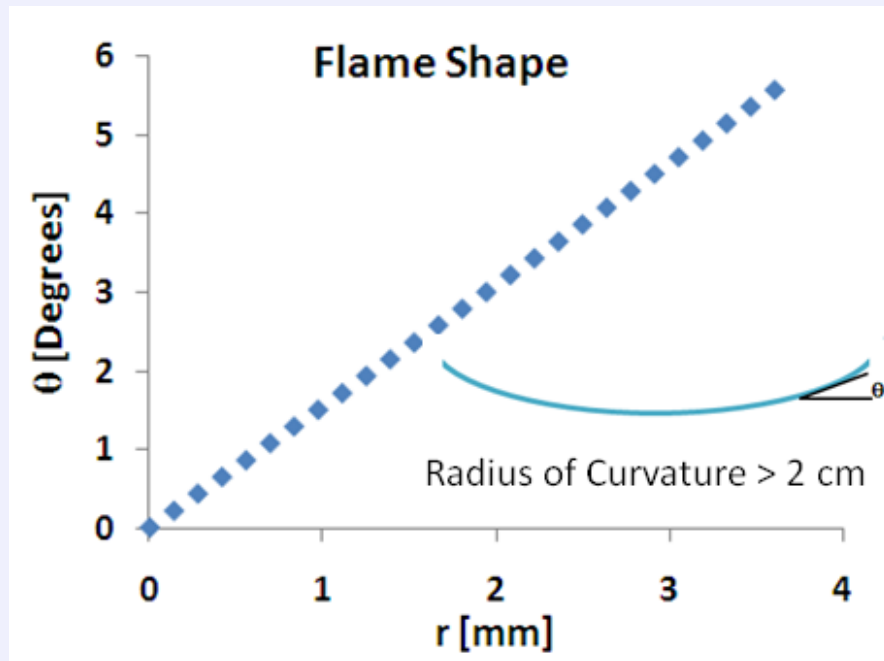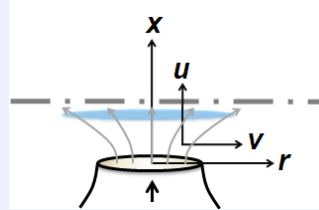
Flame is not perfectly flat, it has curvature that increases away from the centerline
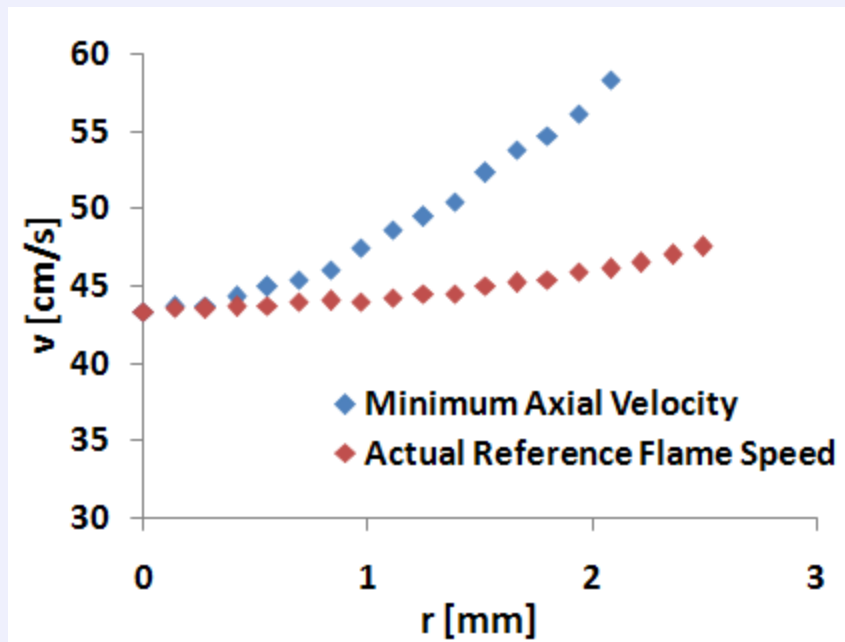
Due to flame curvature, the minimum axial velocity is not the true flame speed away from the centerline. However, the flame speed can be obtained as the component of minimum total velocity normal to the flame surface
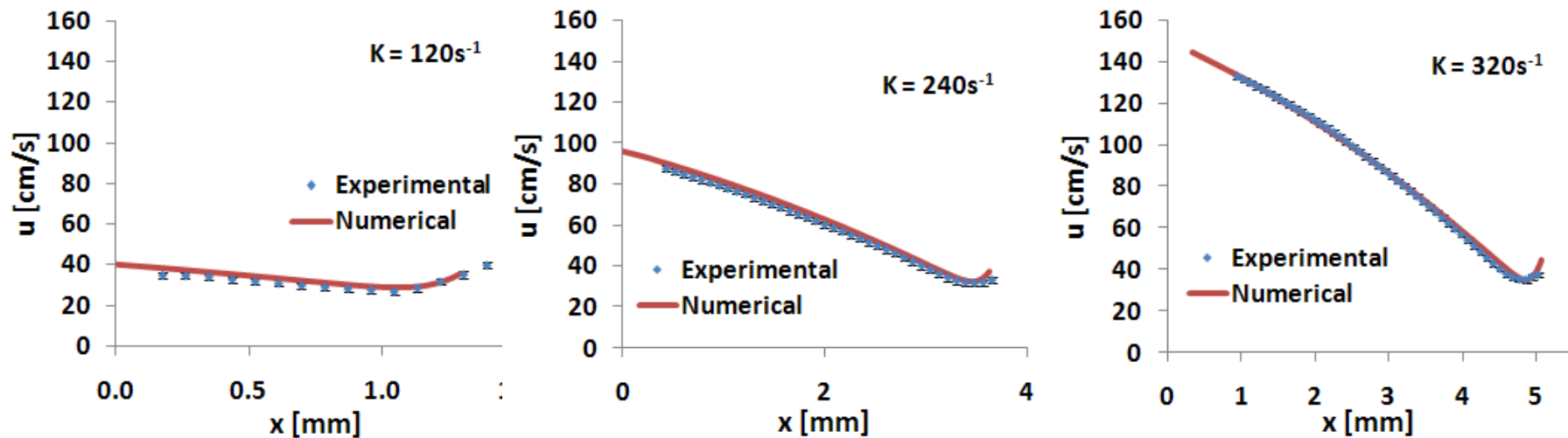
o **Experimental evidence**

Methane/Air, $\phi = 0.8$
Simulations using GRI 3.0

By matching the experimental and numerical strain rates imposed on a flame, the shape of profiles become identical upon translation, proving that the flame is governed by the upstream strain rate

o **Experimental evidence**

C$_2$H$_4$/Air Flames
Simulations using USC Mech II
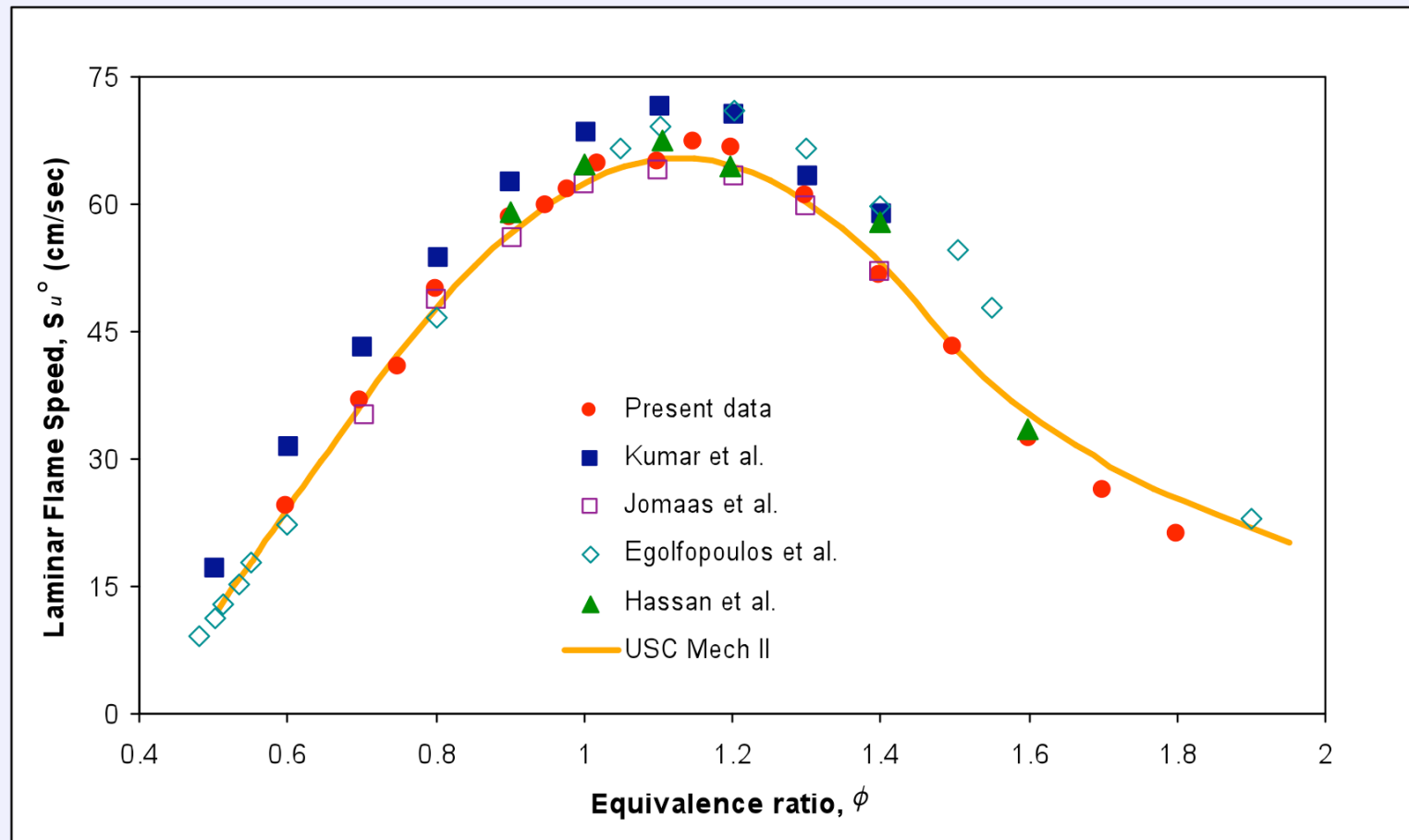
Egolfopoulos, F.N., Zhu, D.L., and Law, C.K., *Proc. Combust. Inst.* 1990, 23, 471.
Hassan, M. I., Aung, K. T., Kwon, K. C., and Faeth, G. M. *J. Propul. Power* 1994, 14, 479.
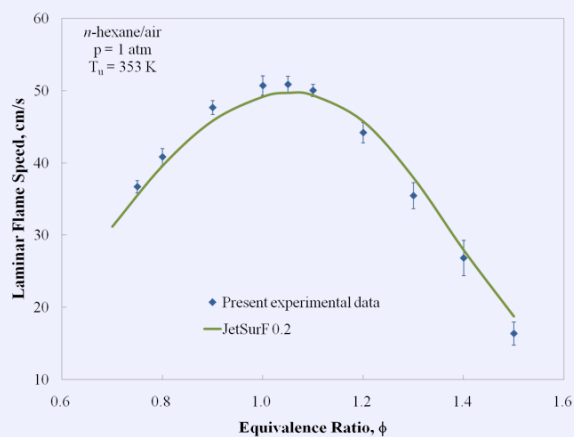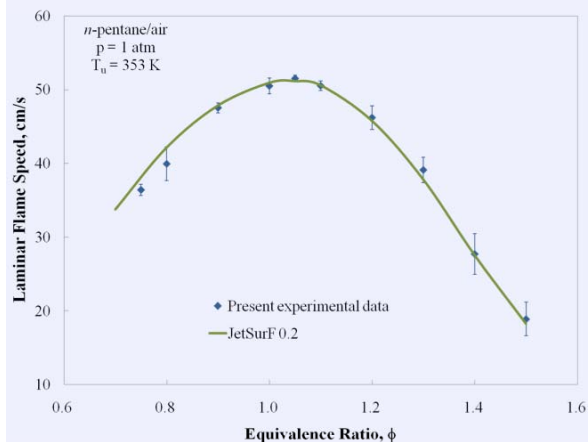Jomaas, G., Zheng, X. L., Zhu, D. L., and Law, C. K., *Proc. Combust. Inst.* 2005, 30, 193
Kumar, K., Mittal, G., Sung, C., Law, C.K., *Combustion and Flame* 153 (2008) 343-354

Propagation and Extinction of

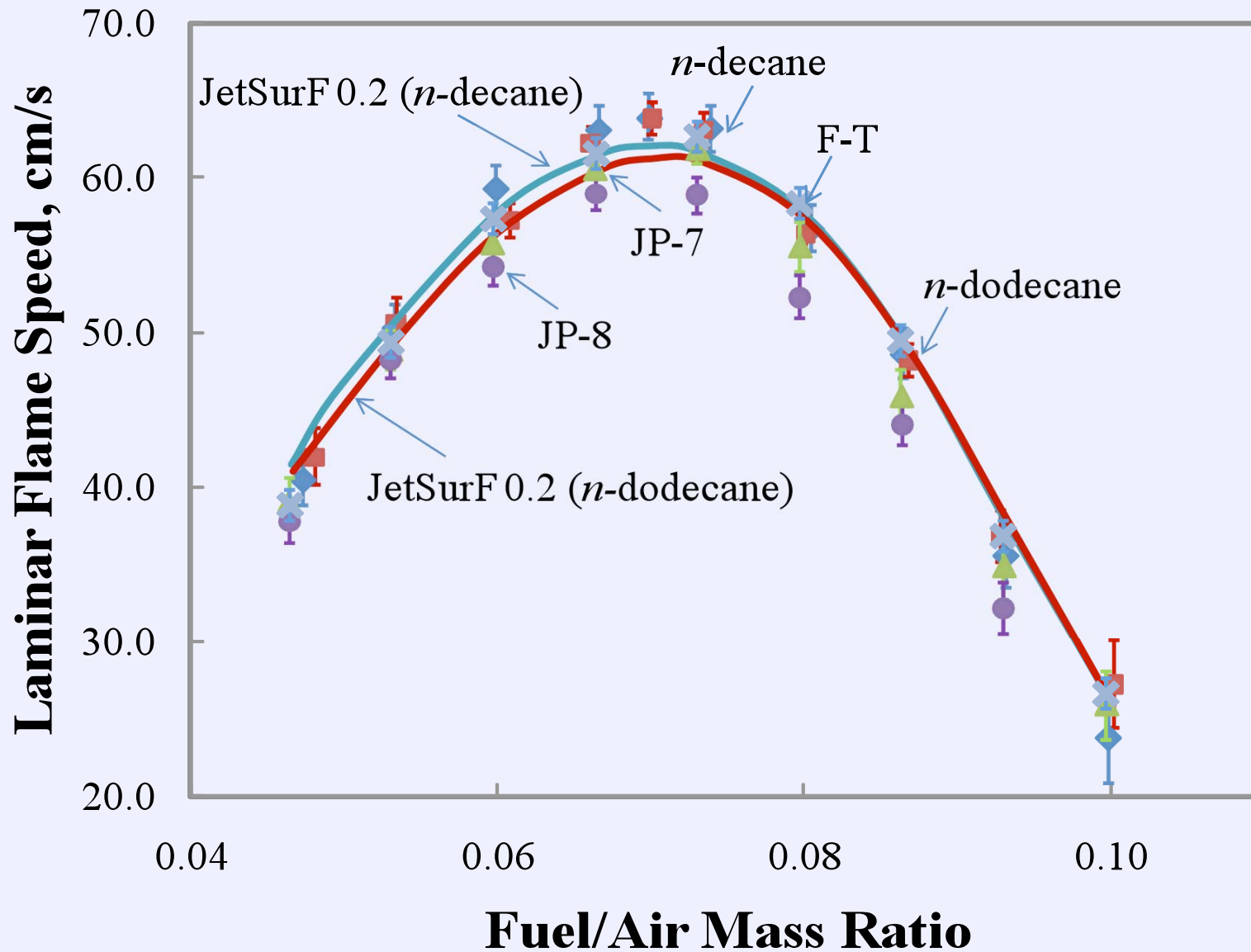# n-Alkane/Air, JP-7/Air, and JP-8/Air Flames

Laminar Flame Speeds of C_5-C_{12} n-Alkane/Air Flames[1]

Laminar Flame Speeds of JP-7 and JP-8 Flames

Extinction Strain Rates of C_5-C_{12} n-Alkane/Air Flames[1]
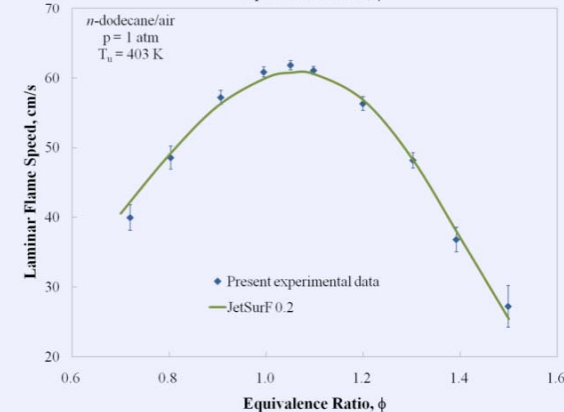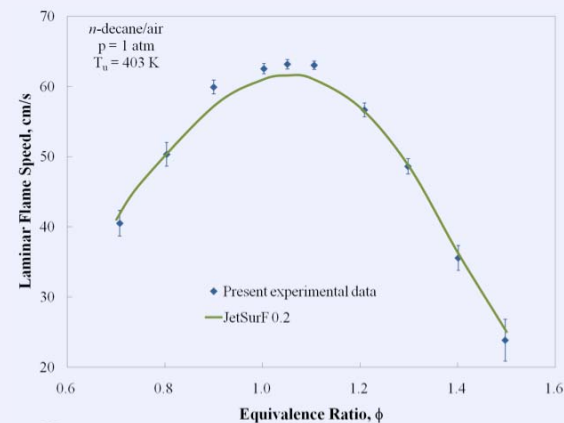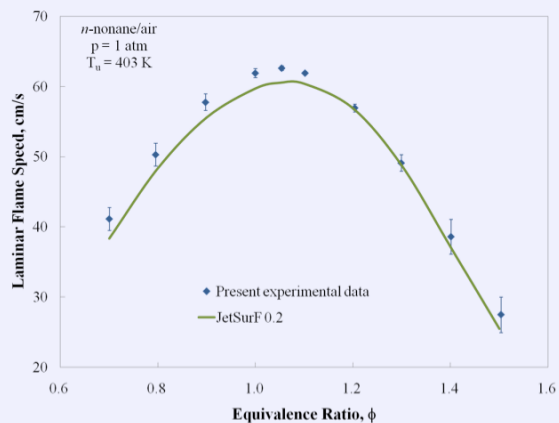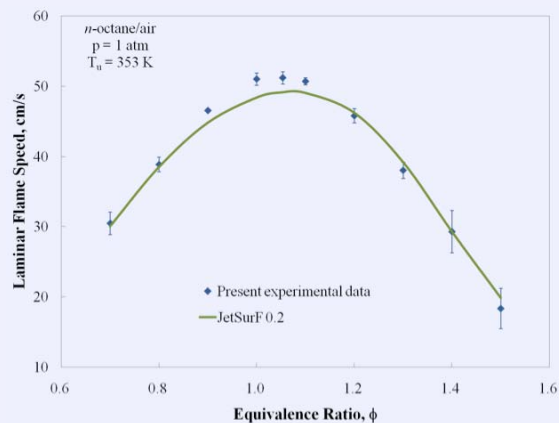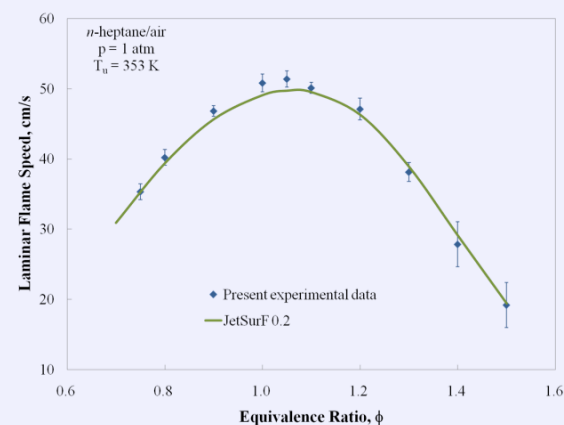
[1]C. Ji, E. Dames, Y.L. Wang, H. Wang, F.N. Egolfopoulos, "Propagation and Extinction of Premixed C_5-C_{12} n-Alkane Flames," Combustion and Flame, doi:10.1016/j.combustflame.2009.06.011, 2009.
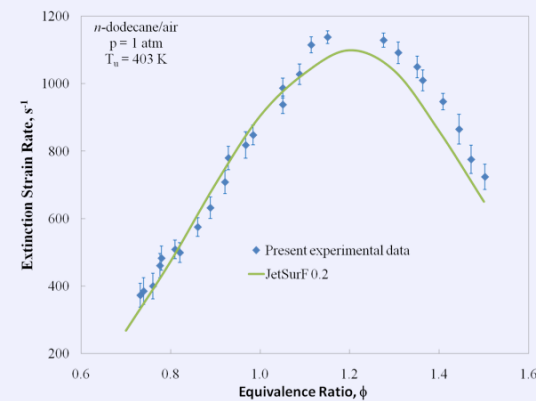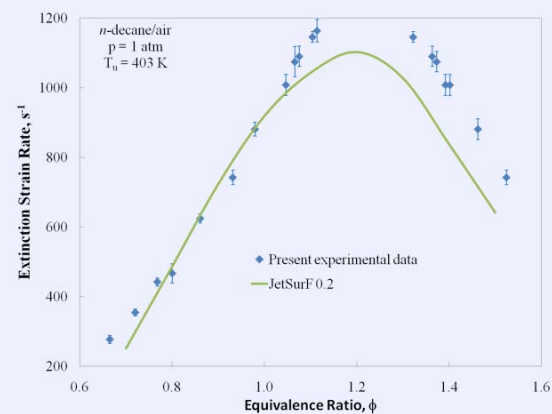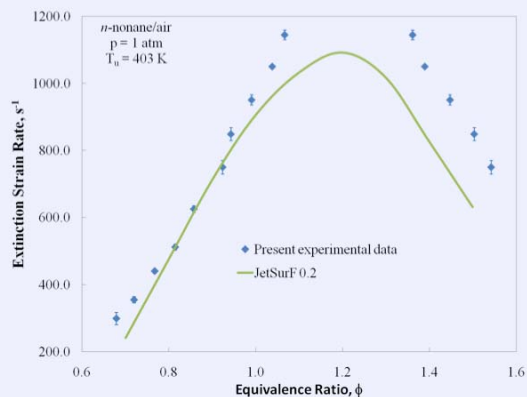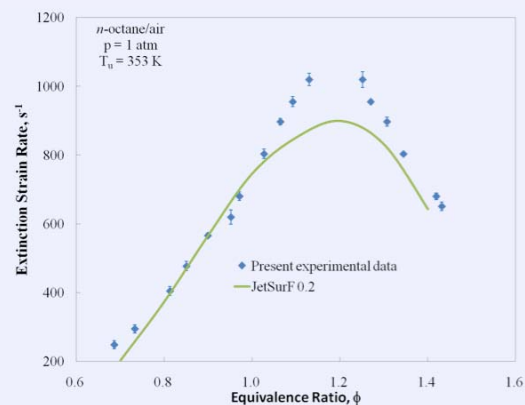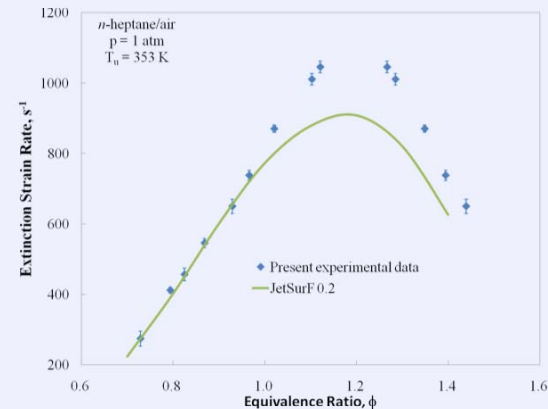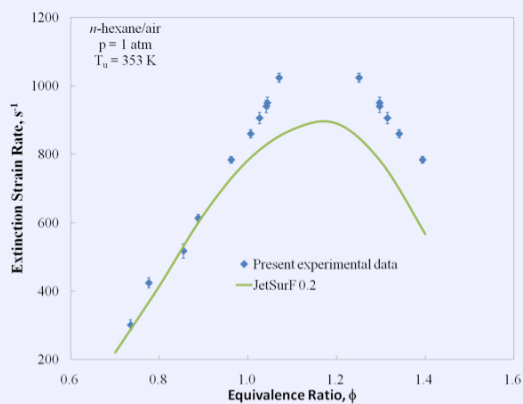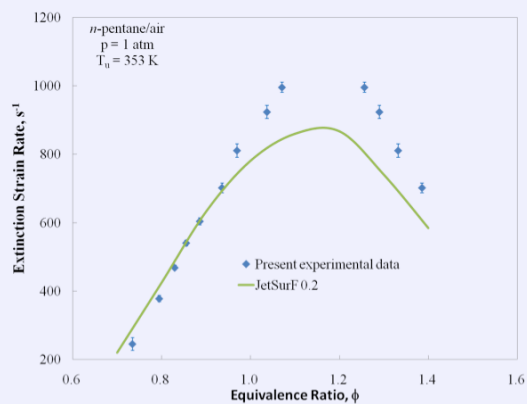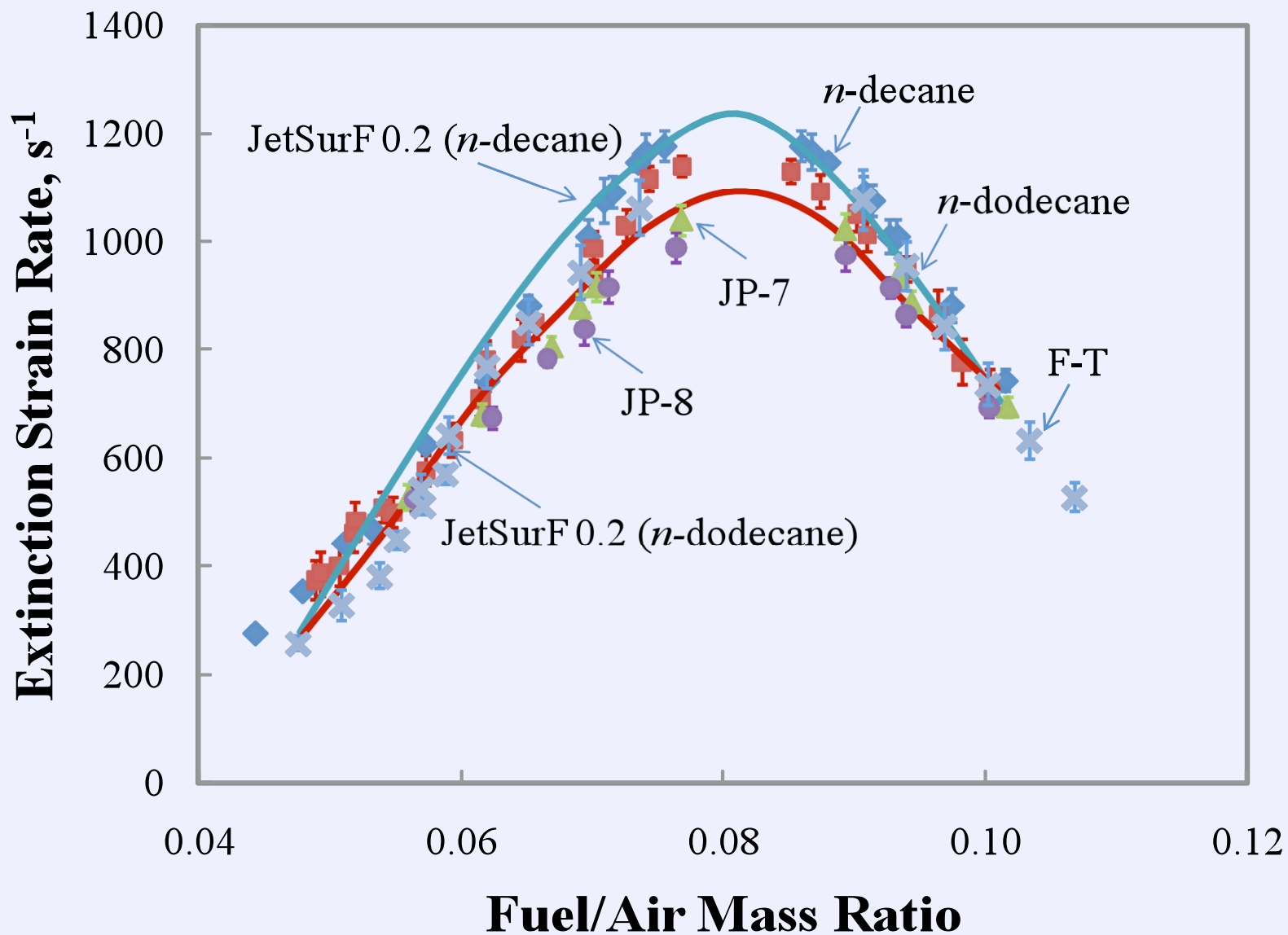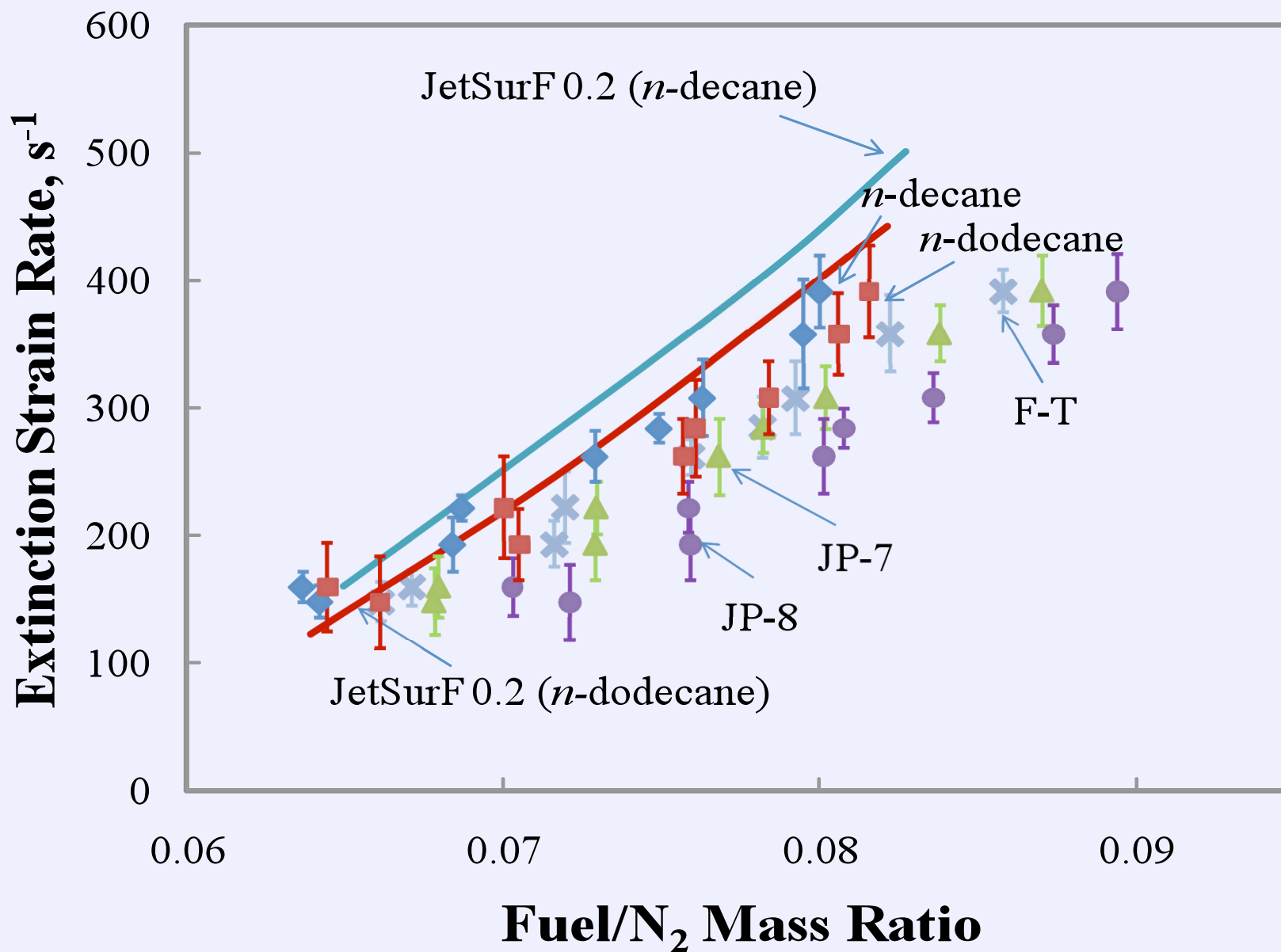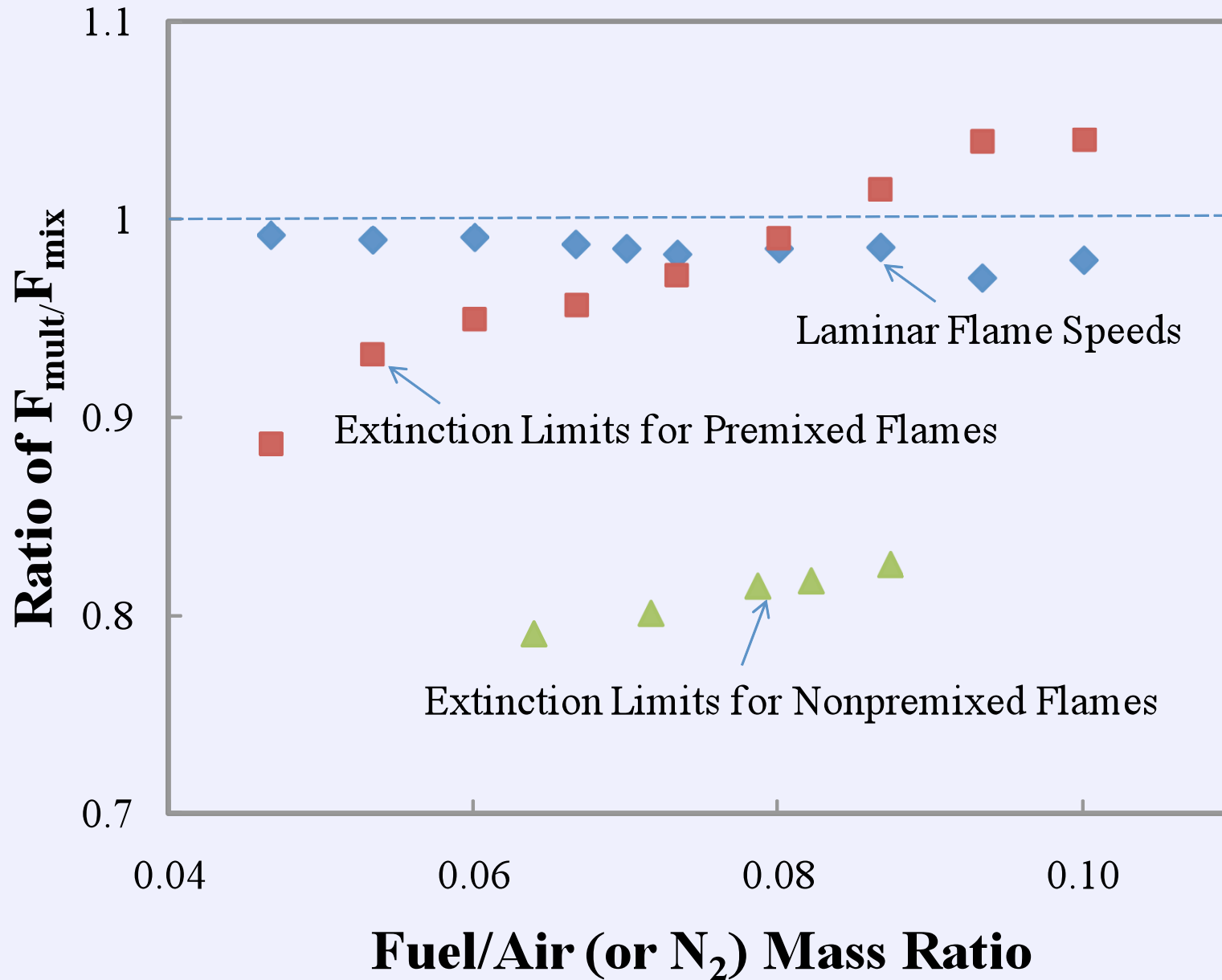
Extinction Strain Rates of JP7 and JP8 Flames

Extinction Strain Rates of Non-Premixed Flames

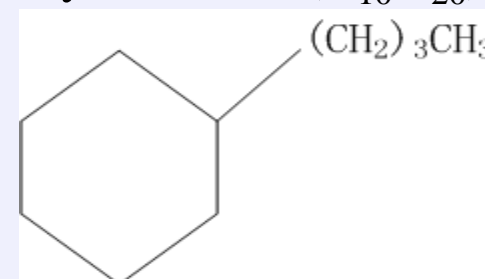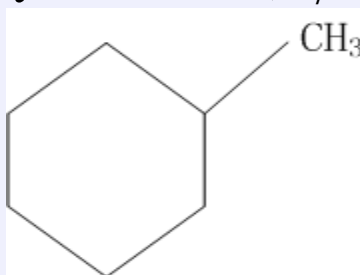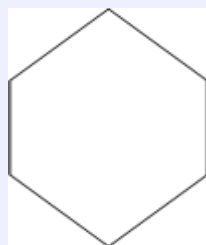**Effect of Transport Formulation on Computed Results**

Propagation and Extinction of

Cycloalkane/Air Flames

Laminar Flame Speeds of Cyclo-Alkane/Air Flames

Cyclohexane(C_6H_{12}): *methyl*-Cyclohexane(C_7H_{14}): *n-butyl*-Cyclohexane($C_{10}H_{20}$):

Experimental configuration:

- Counterflow configuration
- Unburned gas temperature: 80 ^oC
- Ambient pressure

Numerical approach:

- PREMIX and Opposed Jet Code
- Mechanisms:
- **Dagaut** [1]: 209 species, 1673 reactions
        (C_6H_{12})
- **Westbrook** [2]: 1081 species, 4269 reactions
        DRG to: 206 species, 1044 reactions
        (C_6H_{12})
- **JetSurF 1.1** [3]: 350 species, 2094 reactions
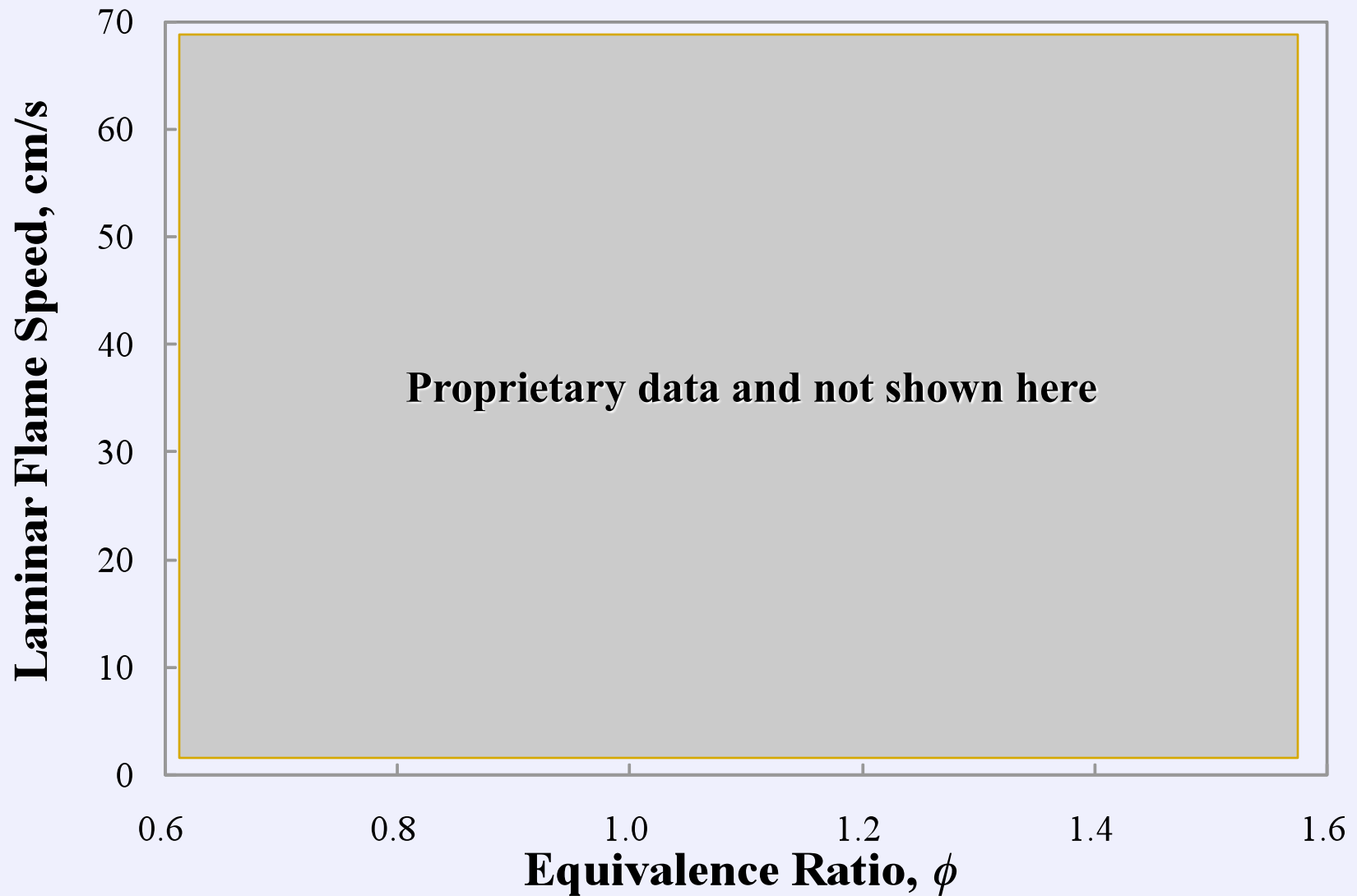   (C_6H_{12}, C_7H_{14}, $C_{10}H_{20}$)

[1] P. Dagaut, M. Cathonnet, *Prog. In Energy and Comb. Sci.* 32 (2006) 48-92
[2] E. J. Silke, W. J. Pitz, C. K. Westbrook and M. Ribaucour, *J. Phys. Chem.A* 111 (2007) 3761-3775
[3] http://melchior.usc.edu/JetSurF/ Released on September 15, 2009

Decomposition of CHX (100)

	JetSurF1.1	Dagaut	Westbrook
C_6H_{11}	56.0	94.3	61.0
C_4H_9	7.5	/	/
C_3H_7	37.4	/	/
C_3H_6	17.0	/	39.0
C_3H_5	22.4	/	/
C_2H_4	7.5	16.5	58.5

Kinetic Effects on the Propagation of Cyclohexane/Air Flames Based on JetSurF 1.1
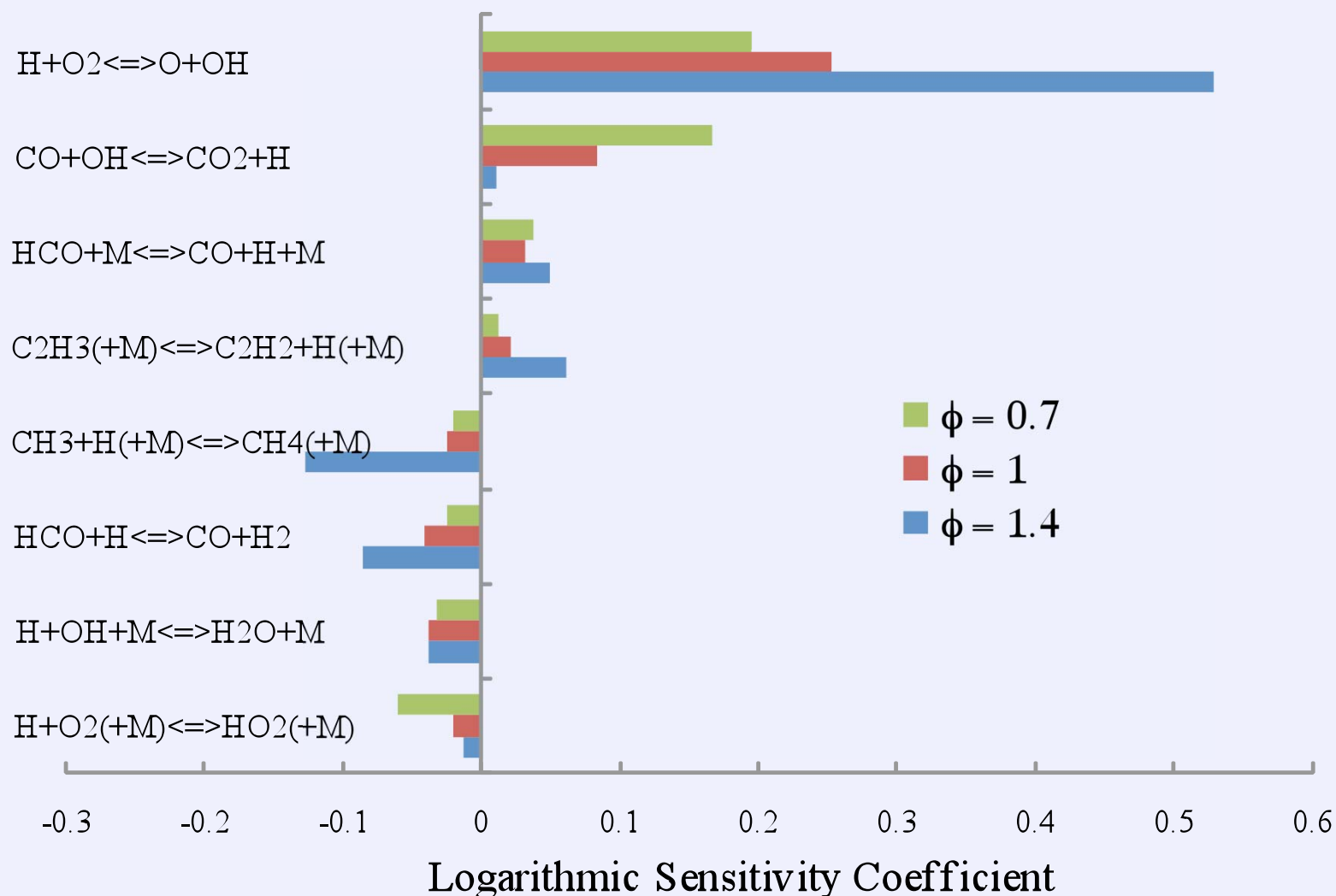
Laminar Flame Speed, cm/s
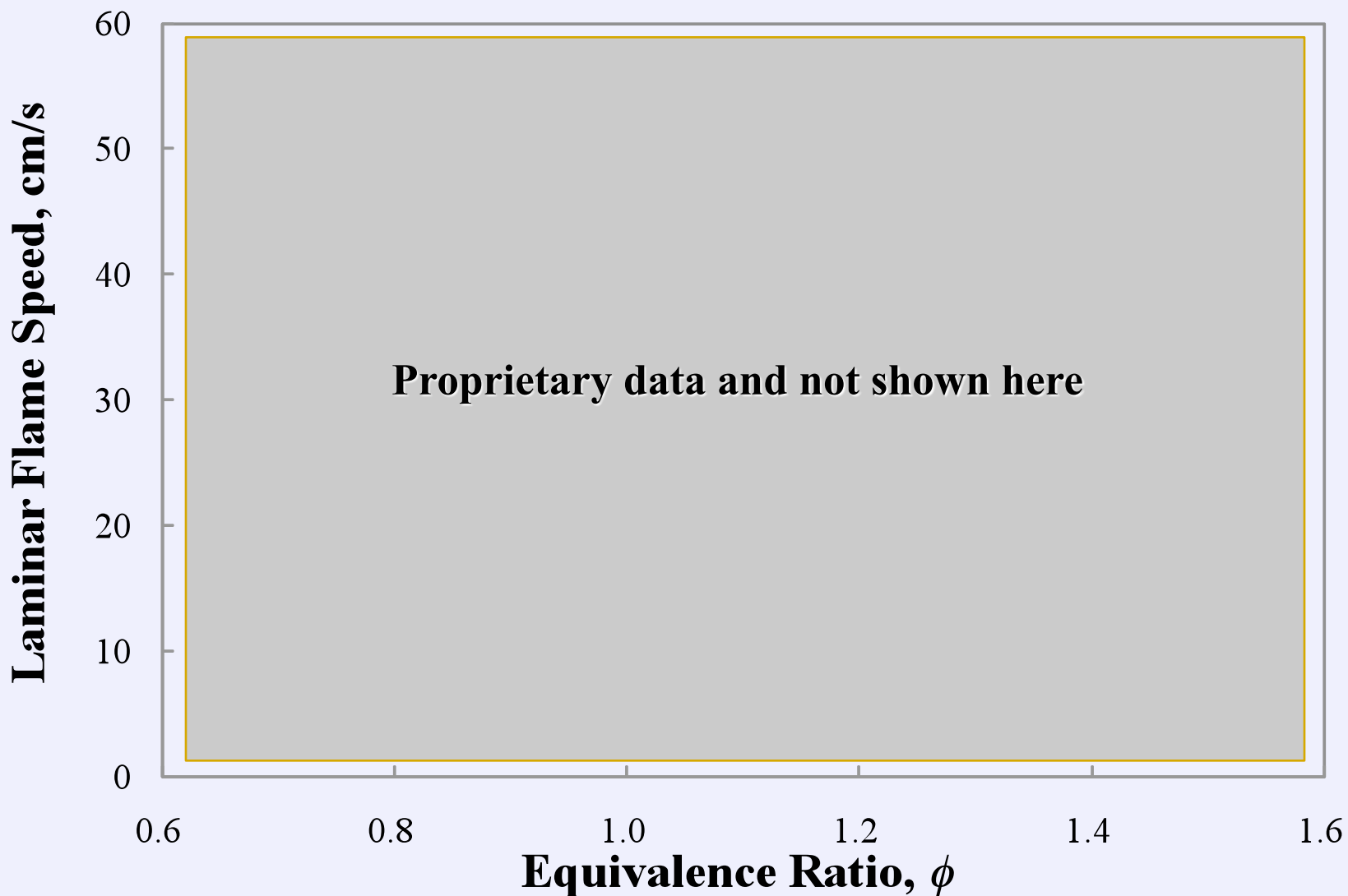
60

50

40

30

Proprietary data and not shown here

20

10

0

0.6   0.8   1.0   1.2   1.4   1.6

Equivalence Ratio, ϕ

Proprietary data and not shown here

Laminar Flame Speed, cm/s vs Equivalence Ratio, ϕ

Laminar Flame Speeds of Cyclo-Alkane/Air Flames

Cyclohexane > *n*-hexane > *n*-butyl-cyclohexane > methyl-cyclohexane

Proprietary data and not shown here

Laminar Flame Speed, cm/s

Equivalence Ratio, ϕ
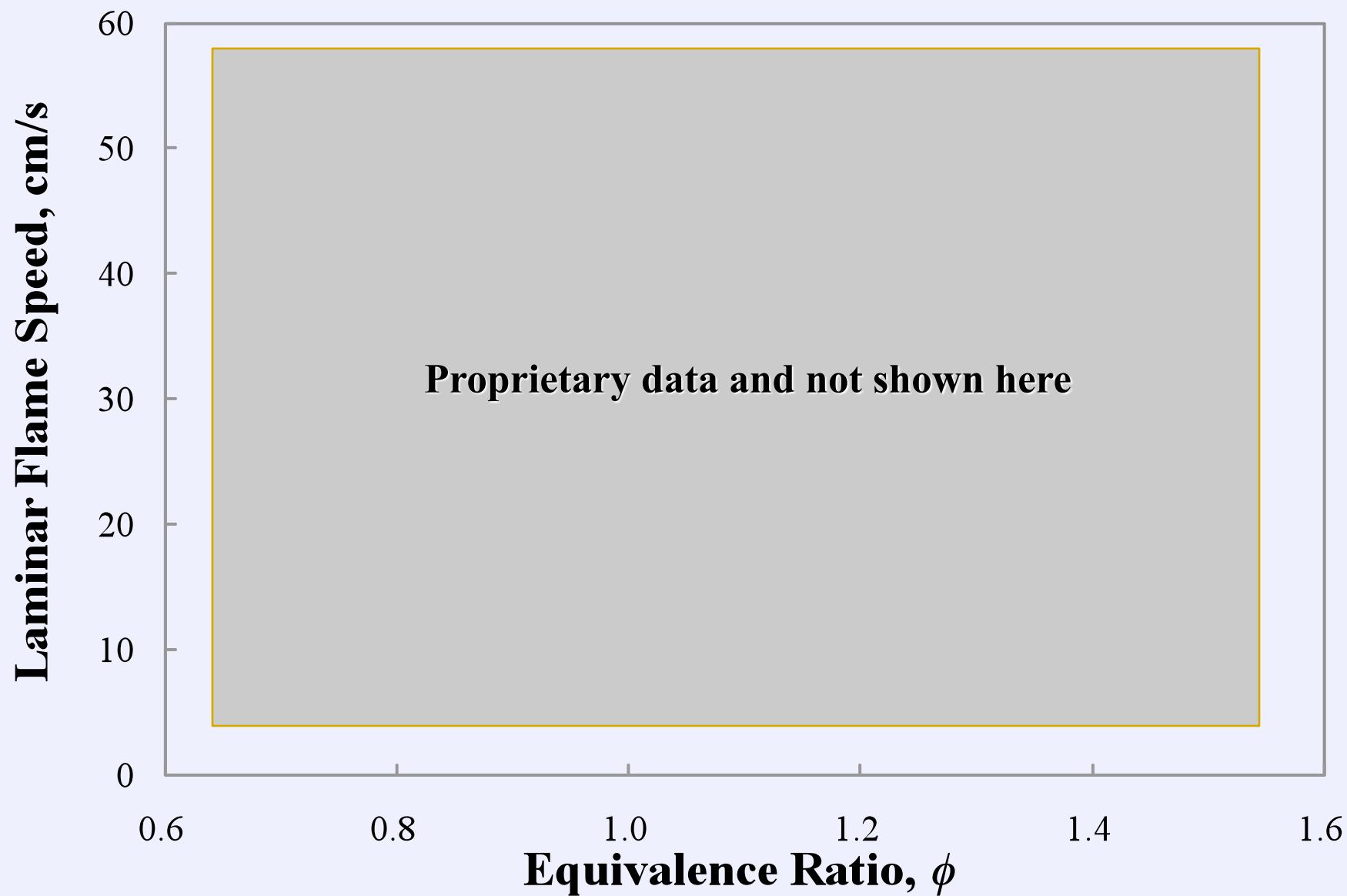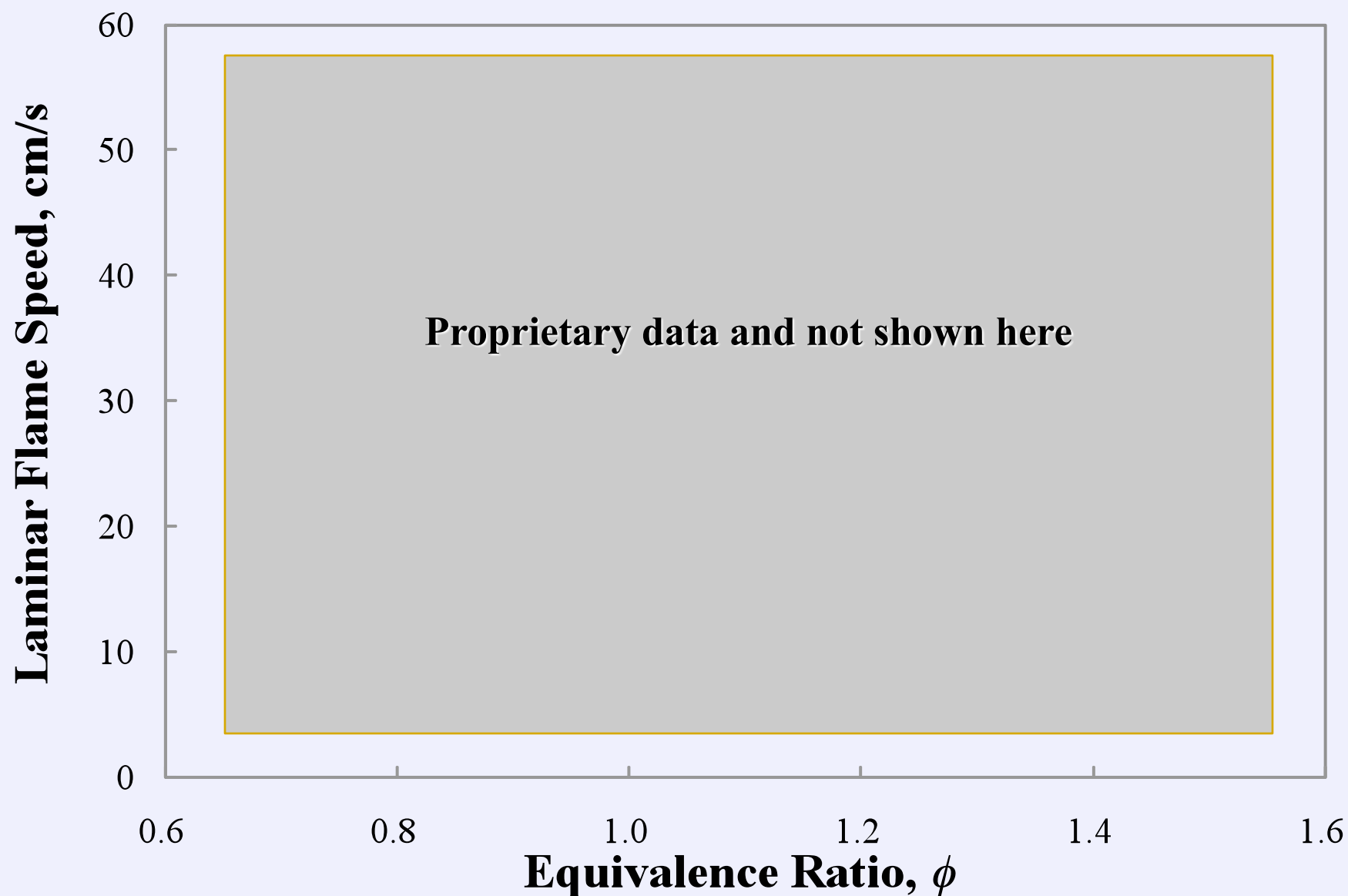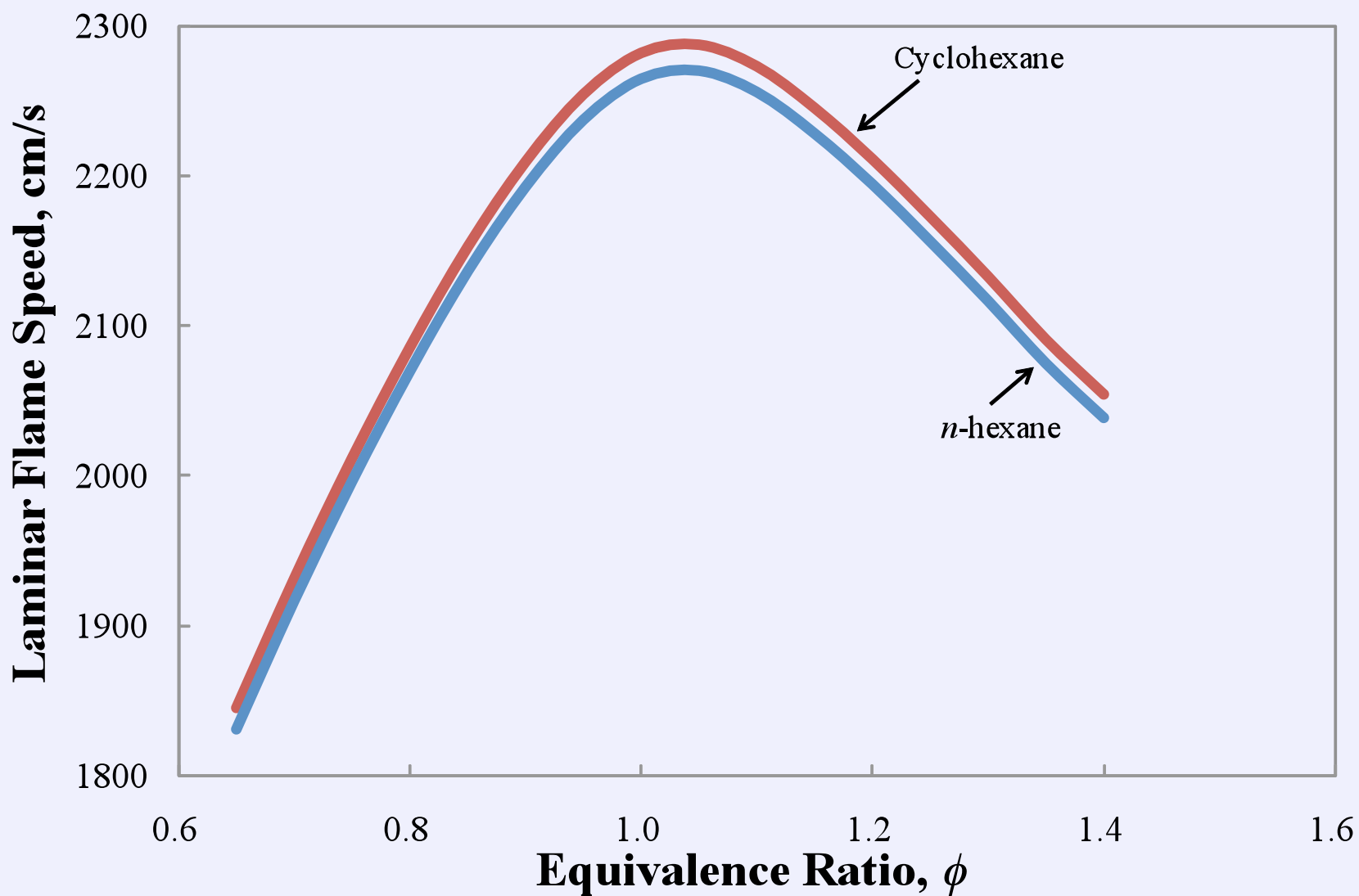
Extinction Strain Rates of Cyclohexane/Air Flames

Extinction Strain Rate, s^{-1}

Proprietary data and not shown here

1000

800

600

400

200

0.6   0.8   1   1.2   1.4   1.6

Equivalence Ratio, ϕ
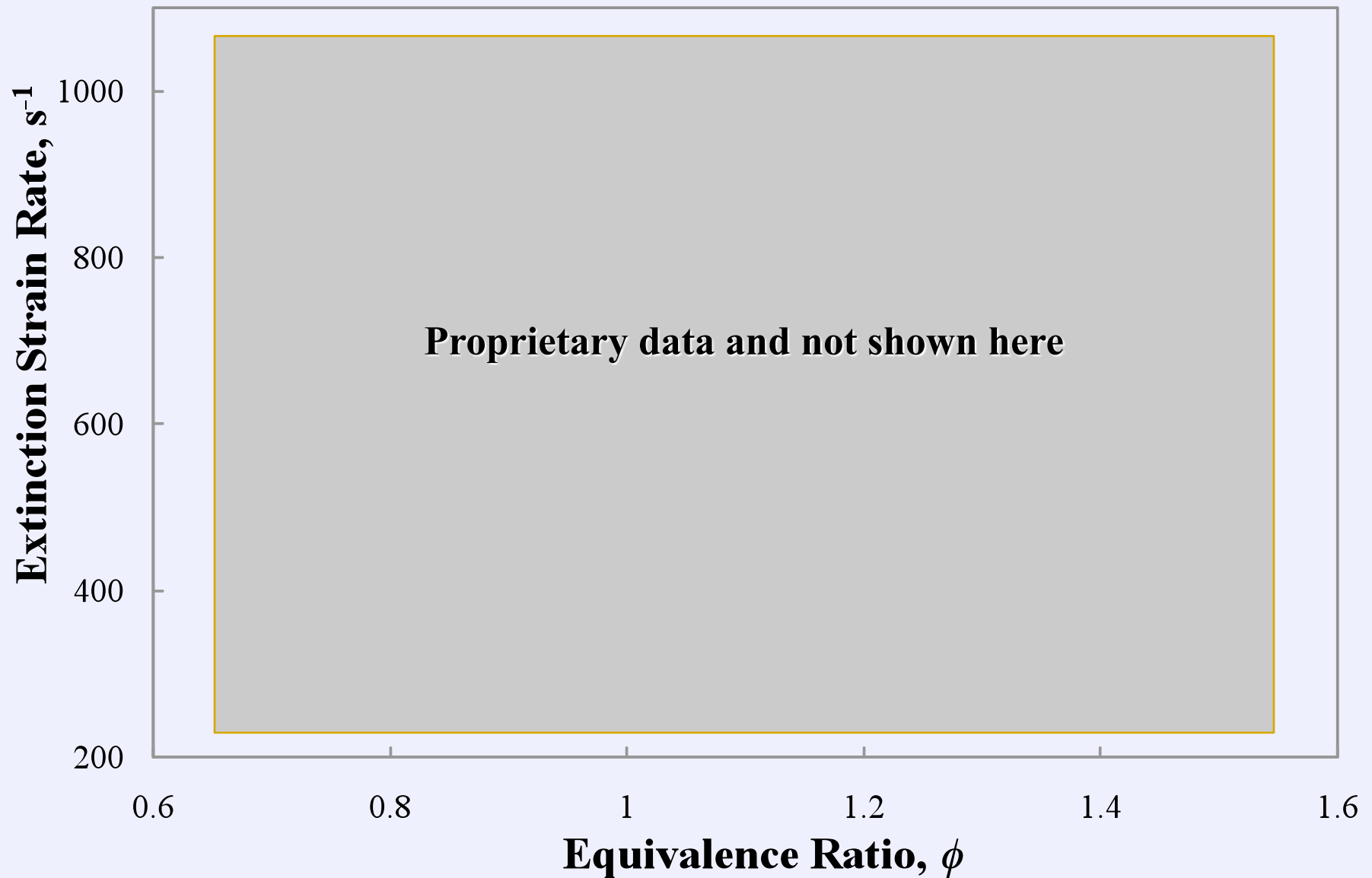
Extinction Strain Rates: Comparisons

Cyclohexane ≥ *n*-hexane > *n*-butyl-cyclohexane > methyl-cyclohexane

Proprietary data and not shown here

Extinction Strain Rate, s^{-1}

Equivalence Ratio, ϕ
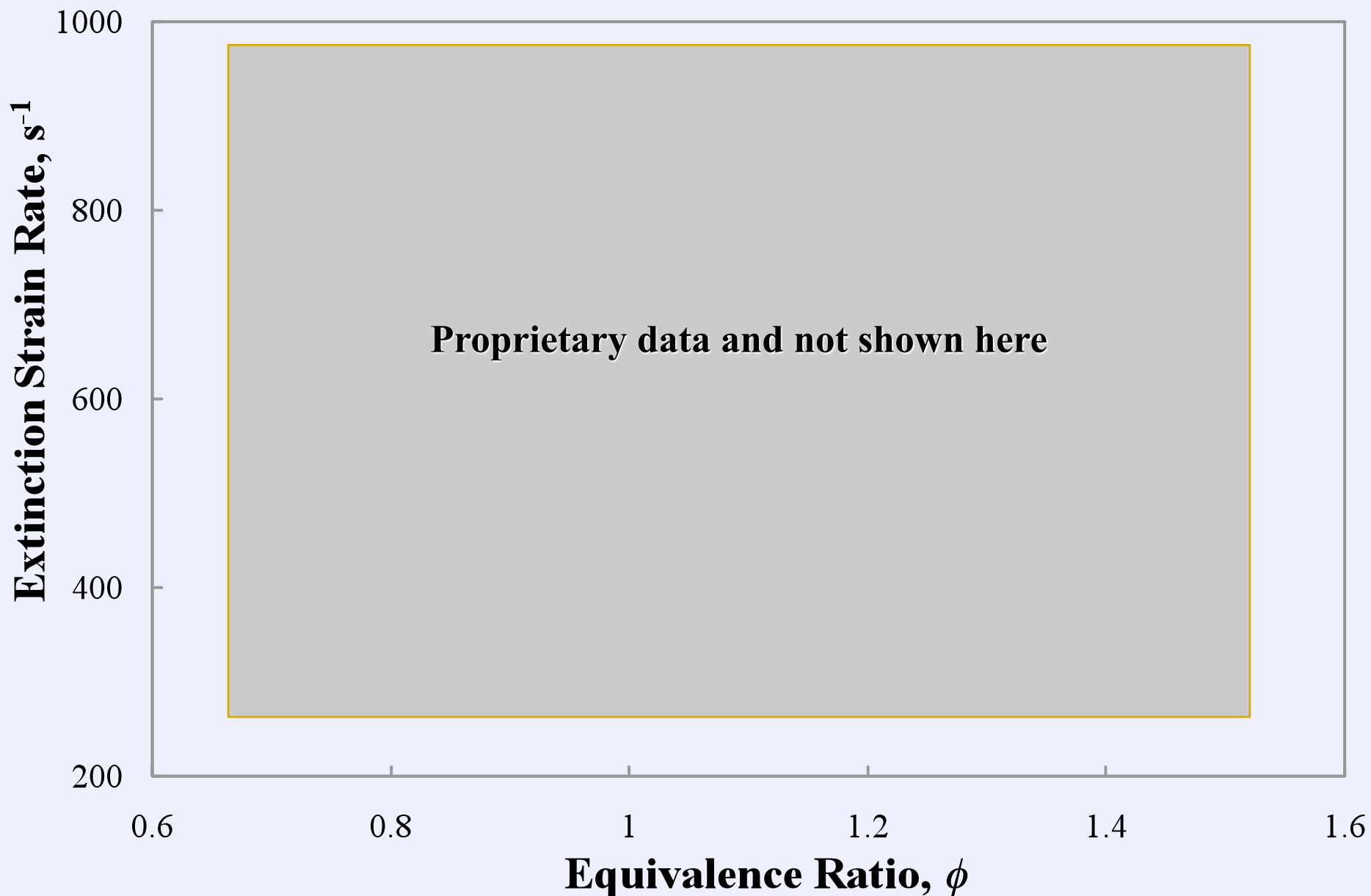
1. The new approach for determining laminar flame speeds using properly computed non-linear extrapolation curves has been evaluated based on additional experimental, theoretical, and numerical evidence.

2. Laminar flame speeds and extinction strain rates have been determined experimentally for atmospheric flames of C_5-C_{12} n-alkanes, selected cycloalkane and aromatic compounds, and JP-7, JP-8, and F-T jet fuels.

3. Flame ignition and elevated pressure propagation and extinction studies have been initiated.

4. A n-dodecane/n-butyl-cyclohexane kinetic model has been advanced and tested against the experimental data and close agreements were found.

5. Under certain conditions the effect of diffusion on the flame response has been found to be of the same magnitude with that of kinetics.

6. *Flame experiments require particular care to overcome inherent challenges and model validation must account for both kinetics and transport effects*